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FILE COVERS 1907-1966
FILE LAST UPDATED: 01 May 1997 (19970501/UP)

This file contains CAS Registry Numbers for easy and accurate substance identification. Title keywords, authors, patent assignees, and patent information, e.g., patent numbers, are now searchable from 1907-1966. TIFF images of CA abstracts printed between 1907-1966 are available in the PAGE display formats.

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(FILE 'HOME' ENTERED AT 15:47:41 ON 07 SEP 2004)

FILE 'REGISTRY' ENTERED AT 15:47:49 ON 07 SEP 2004
L1 STRUCTURE UPLOADED
L2 9 S L1
L3 659 S L1 FULL

FILE 'HCAPLUS' ENTERED AT 15:53:02 ON 07 SEP 2004
L4 182 S L3

FILE 'REGISTRY' ENTERED AT 15:53:30 ON 07 SEP 2004
L5 STRUCTURE UPLOADED
L6 8 S L5
L7 640 S L5 FULL

FILE 'HCAPLUS' ENTERED AT 15:54:31 ON 07 SEP 2004
L8 177 S L7

FILE 'REGISTRY' ENTERED AT 15:55:15 ON 07 SEP 2004
L9 STRUCTURE UPLOADED
L10 16 S L9
L11 498 S L10 FULL

FILE 'HCAPLUS' ENTERED AT 15:59:33 ON 07 SEP 2004
L12 162 S L11
L13 0 S L12 AND LU, Z?/AU
L14 0 S L12 AND MADUSKUIE, T?/AU
L15 0 S L12 AND VOSS, M?/AU
L16 0 S L12 AND DUAN, J?/AU
L17 0 S L12 AND OTT, G?/AU
L18 0 S L1

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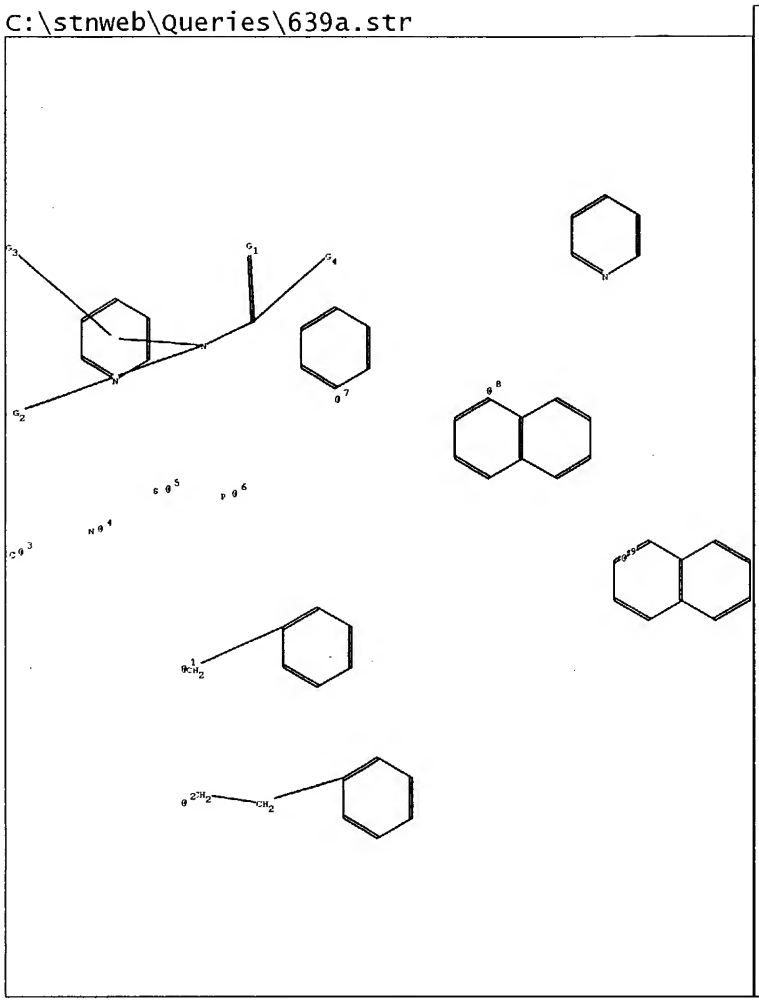

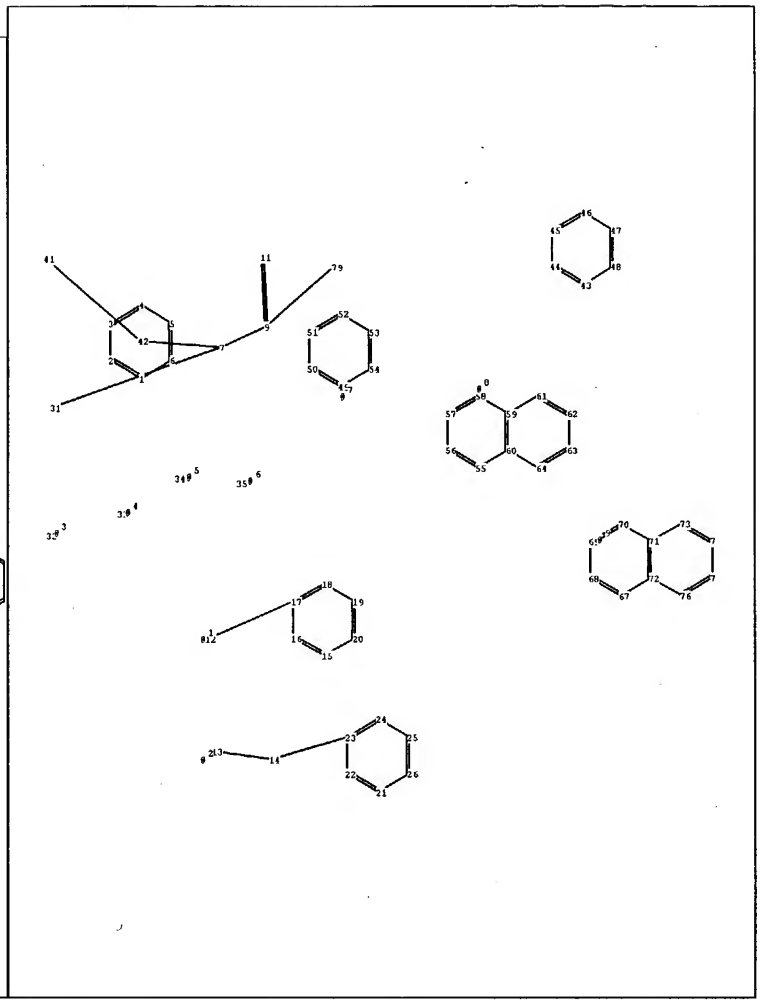

chain nodes :
7 9 11 12 13 14 31 32 33 34 35 41 79
ring nodes :
1 2 3 4 5 6 15 16 17 18 19 20 21 22 23 24 25 26 43 44 45 46 47 48
49 50 51 52 53 54 55 56 57 58 59 60 61 62 63 64 67 68 69 70 71 72
73 74 75 76
chain bonds :
7-9 7-31 9-11 9-79 12-17 13-14 14-23
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 15-16 15-20 16-17 17-18 18-19 19-20 21-22 21-26
22-23 23-24 24-25 25-26 43-44 43-48 44-45 45-46 46-47 47-48 49-50 49-54 50-51
51-52 52-53 53-54 55-56 55-60 56-57 57-58 58-59 59-60 59-61 60-64 61-62 62-63
63-64 67-68 67-72 68-69 69-70 70-71 71-72 71-73 72-76 73-74 74-75 75-76
exact/norm bonds :
7-9 7-31 9-11 9-79
exact bonds :
12-17 13-14 14-23
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 15-16 15-20 16-17 17-18 18-19 19-20 21-22 21-26
22-23 23-24 24-25 25-26 43-44 43-48 44-45 45-46 46-47 47-48 49-50 49-54 50-51
51-52 52-53 53-54 55-56 55-60 56-57 57-58 58-59 59-60 59-61 60-64 61-62 62-63
63-64 67-68 67-72 68-69 69-70 70-71 71-72 71-73 72-76 73-74 74-75 75-76
isolated ring systems :
containing 15 : 21 : 43 : 49 : 55 : 67 :

G1:O,S

G2:H,Ph,Ak,[*1],[*2]

G3:[*1],[*2],[*3],[*4],[*5],[*6]

G4:[*7],[*8],[*9]

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 11:CLASS
12:CLASS 13:CLASS 14:CLASS 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom
21:Atom 22:Atom 23:Atom 24:Atom 25:Atom 26:Atom 31:CLASS 32:CLASS 33:CLASS
34:CLASS 35:CLASS 41:CLASS 42:CLASS 43:Atom 44:Atom 45:Atom 46:Atom 47:Atom
48:Atom 49:CLASS 50:CLASS 51:Atom 52:Atom 53:Atom 54:Atom 55:Atom 56:Atom
57:Atom 58:Atom 59:Atom 60:Atom 61:Atom 62:Atom 63:Atom 64:Atom 67:Atom 68:Atom
69:Atom 70:Atom 71:Atom 72:Atom 73:Atom 74:Atom 75:Atom 76:Atom 79:CLASS

WO 2002010154	A2	20020207	WO 2001-US16528		20010718
WO 2002010154	A3	20020627			
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM					
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG					
EP 1307444	A2	20030507	EP 2001-958825		20010718
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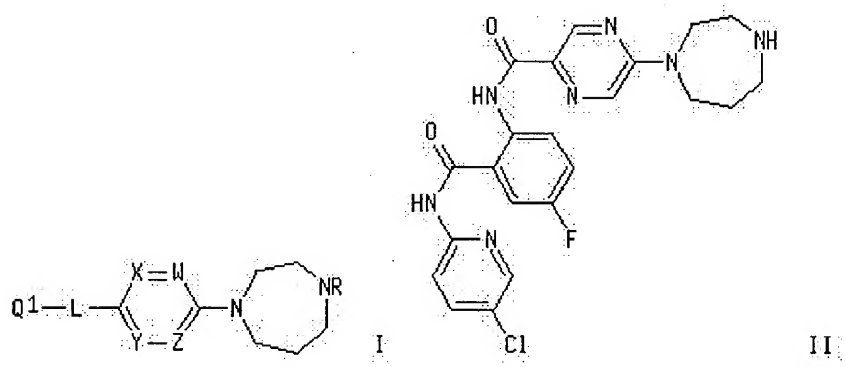
US 2004097491	A1	20040520	US 2003-332120		20030102
PRIORITY APPLN. INFO.:			US 2000-221092P	P	20000727
			WO 2001-US16528	W	20010718

OTHER SOURCE(S): MARPAT 136:151189

GI



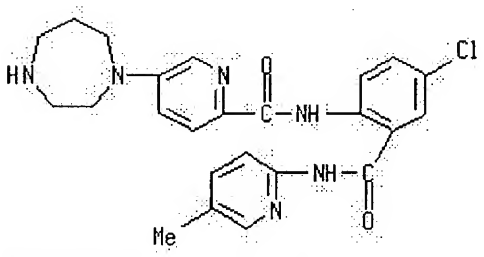
AB Substituted hexahydrodiazepines I [R = H, alkyl, acyl, acetyloxy, acetyl, aminoacetyl, alkylamido, etc.; one or two of X, W, Y, and Z equals N and each of the others of X, W, Y and Z is CH; when L = CO or CH2, Q1 = (un)substituted pyridinyl- or phenyl-amidophenylamine, in addn. when L = CO, Q1 may equal Q2X2SO2N(CH2CH2)2N- wherein Q2 = (un)substituted Ph, benzo[b]thiophen-2-yl or naphthalen-2-yl (X2 = direct bond, CH2, ethylene, or ethen-1,2-diyl)], and their pharmaceutically acceptable salts are prepd. and disclosed as factor Xa inhibitors. Thus, II was prepd. by amidation of 2-amino-5-fluoro-N-(5-chloropyridin-2-yl)benzamide with 5-hydroxy-pyrazine-2-carboxylic acid (via its acid chloride) followed by substitution with 1-BOC-hexahydro-1,4-diazepine and subsequent deprotection of the diazepinyl nitrogen. As factor Xa inhibitors, the compds. of the invention are claimed to be useful in the treatment of thromboembolic disorders (no data).

IT **395683-78-0P**

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(prepn. of pyrazinyl-, pyridazinyl-, pyrimidinyl-, and

h eb c g cg b cg eb

pyridinyl-hexahydrodiazepines as factor Xa inhibitors)
RN 395683-78-0 HCAPLUS
CN 2-Pyridinecarboxamide, N-[4-chloro-2-[[(5-methyl-2-pyridinyl)amino]carbonyl]phenyl]-5-(hexahydro-1H-1,4-diazepin-1-yl)- (9CI) (CA INDEX NAME)



L12 ANSWER 41 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

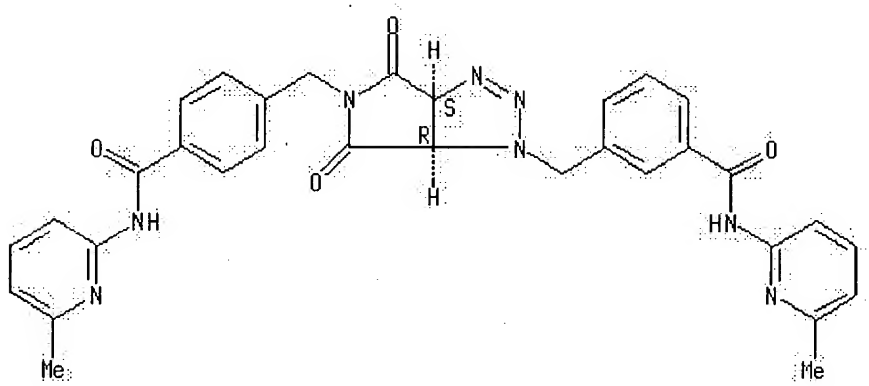
Full Text | Citing Ref. | Related Records

ACCESSION NUMBER: 2002:14174 HCAPLUS
DOCUMENT NUMBER: 136:216362
TITLE: A Generic Recognition-Based Approach to the Acceleration of Cycloaddition Reactions
AUTHOR(S): Howell, Sarah J.; Spencer, Neil; Philp, Douglas
CORPORATE SOURCE: Centre for Biomolecular Sciences School of Chemistry, University of St. Andrews, St Andrews, KY16 9ST, UK
SOURCE: Organic Letters (2002), 4(2), 273-276
CODEN: ORLEF7; ISSN: 1523-7060
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Dicarboxylic acids accelerate the rate of cycloaddn. reactions between either an azide or a furan and a maleimide through the formation of a reactive 1:1:1 complex stabilized by four hydrogen bonds.

IT **402750-23-6**
RL: FMU (Formation, unclassified); PRP (Properties); FORM (Formation, nonpreparative)
(recognition-based approach to acceleration of cycloaddn. reactions)
RN 402750-23-6 HCAPLUS
CN Benzamide, N-(6-methyl-2-pyridinyl)-3-[[(3aR,6aS)-4,5,6,6a-tetrahydro-5-[[4-[[(6-methyl-2-pyridinyl)amino]carbonyl]phenyl]methyl]-4,6-dioxopyrrolo[3,4-d]-1,2,3-triazol-1(3aH)-yl]methyl]-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



h eb c g cg b cg eb

REFERENCE COUNT: 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 42 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Linked References

ACCESSION NUMBER: 2002:11104 HCAPLUS
DOCUMENT NUMBER: 136:69743
TITLE: Preparation of pyridyl benzamides and related compounds as Factor Xa inhibitors.
INVENTOR(S): Zhu, Bing-Yan; Zhang, Penglie; Wang, Lingyan; Huang, Wenrong; Goldman, Erick A.; Li, Wenhao; Zuckett, Jingmei; Song, Yonghong; Scarborough, Robert
PATENT ASSIGNEE(S): USA
SOURCE: U.S. Pat. Appl. Publ., 259 pp., Cont.-in-part of U.S. Ser. No. 663,420.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 6
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
US 2002002183	A1	20020103	US 2001-794225		20010228
US 6376515	B2	20020423			
US 2003162690	A1	20030828	US 2002-126976		20020422
US 2004097561	A1	20040520	US 2003-687334		20031015
PRIORITY APPLN. INFO.:			US 2000-185746P	P	20000229
			US 2000-663420	A2	20000915
			US 2001-794225	A1	20010228
			US 2002-126976	A1	20020422

OTHER SOURCE(S): MARPAT 136:69743

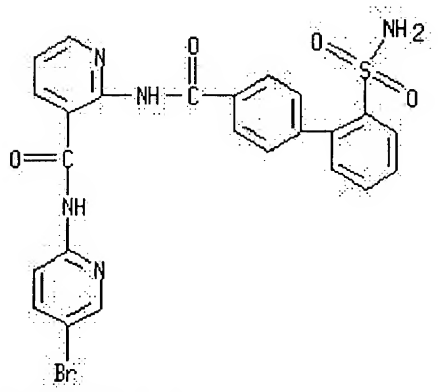
AB AQDEGJX [A = alkyl, cycloalkyl, NR1R2, NR1R2C(:NR3), (substituted) Ph, naphthyl, heterocyclyl, etc.; R1-R3 = H, OR5, NR5R6, alkyl, alkenyl, etc.; R1R2 or R2R3 = atoms to form (substituted) cycloalkyl, heterocyclyl; R5, R6 = H, alkyl, alkenyl, alkynyl, cycloalkyl, (substituted) alkylphenyl, alkylnaphthyl; R5R6 = atoms to form a 3-8 membered (substituted) ring; Q = bond, CH2, CO, O, S, SO, SO2, NR7, SO2NR7, etc.; R7 = H, alkyl, alkenyl, alkynyl, cycloalkyl, alkylcycloalkyl, (substituted) alkylphenyl, alkylnaphthyl; D = bond, (substituted) Ph, naphthyl, mono- or bicyclic heterocyclyl; E = bond, alkyl, O, S, SO, SO2, alkylcarbonyl, etc.; G = (substituted) alkenyl, cycloalkenyl, phenylene, 3-8 membered (fused) (arom.) heterocyclyl; J = bond, NR9CO, O, S, SO, SO2, CH2, NR9SO2, etc.; X = (substituted) Ph, naphthyl, (fused) heteroaryl], were prepd. as antithrombotics (no data). Thus, N-(5-bromo-2-pyridinyl)-2-aminophenylcarboxamide (prepn. given), 4-cyanobenzoyl chloride, and pyridine were stirred overnight in CH2Cl2 to give 70% N-(5-bromo-2-pyridinyl)-[2-(4-cyanophenylcarbonyl)amino]phenylcarboxamide. The latter in MeOH at 0° was satd. with HCl and stirred overnight followed by solvent evapn. The residue was refluxed 2 h with NH4OAc in MeOH to give 70% N-(5-bromo-2-pyridinyl)-[2-(4-amidinophenylcarbonyl)amino]phenylcarboxamide.

IT **330939-74-7P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of pyridyl benzamides and related compds. as Factor Xa inhibitors)

RN 330939-74-7 HCAPLUS

h eb c g cg b cg eb

CN 3-Pyridinecarboxamide, 2-[[[2'-(aminosulfonyl)[1,1'-biphenyl]-4-yl]carbonyl]amino]-N-(5-bromo-2-pyridinyl)- (9CI) (CA INDEX NAME)



L12 ANSWER 43 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER:	2001:896753 HCAPLUS
DOCUMENT NUMBER:	136:118326
TITLE:	Molecular recognition of xanthine alkaloids: first synthetic receptors for theobromine and a series of new receptors for caffeine
AUTHOR(S):	Goswami, Shyamaprosad; Mahapatra, Ajit Kumar; Mukherjee, Reshmi
CORPORATE SOURCE:	Department of Chemistry, Bengal Engineering College (Deemed University), Howrah, 711103, India
SOURCE:	Journal of the Chemical Society, Perkin Transactions 1 (2001), (20), 2717-2726 CODEN: JCSPCE; ISSN: 1472-7781
PUBLISHER:	Royal Society of Chemistry
DOCUMENT TYPE:	Journal
LANGUAGE:	English
OTHER SOURCE(S):	CASREACT 136:118326
GI	

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Synthetic receptors [I, II (R = H, Ac) and III] are designed and synthesized for the first time for theobromine, a xanthine alkaloid used as a diuretic. The synthesis of the receptor III is achieved by Co(PPh3)3Cl-mediated homocoupling of 3-(ethoxycarbonyl)benzyl bromide under mild conditions. New caffeine receptors [IV and V (X = CH2, SO2)] are designed and synthesized. The binding results of theobromine and caffeine (both by NMR and UV studies) are reported.

IT **390358-50-6P**

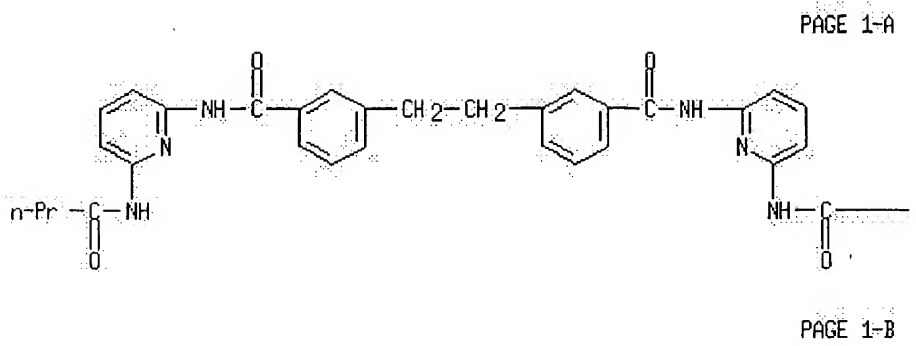
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PYP (Physical process); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); PROC (Process); RACT (Reactant or reagent)

(mol. recognition of xanthine alkaloids by synthetic receptors specific for theobromine or caffeine)

RN 390358-50-6 HCAPLUS

CN Benzamide, 3,3'-(1,2-ethanediyl)bis[N-[6-[(1-oxobutyl)amino]-2-pyridinyl]- (9CI) (CA INDEX NAME)

h eb c g cg b cg eb



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REFERENCE COUNT: 39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 44 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 2001:873334 HCAPLUS
DOCUMENT NUMBER: 136:12632
TITLE: New heterocyclic compound for electroluminescent device
INVENTOR(S): Okada, Hisashi; Ise, Toshihiro
PATENT ASSIGNEE(S): Fuji Photo Film Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 52 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
JP 2001335776	A2	20011204	JP 2000-218967		20000719
US 6461747	B1	20021008	US 2000-621740		20000721
US 2003091861	A1	20030515	US 2002-224377		20020821
US 6656612	B2	20031202			
US 2004062952	A1	20040401	US 2003-671406		20030926
PRIORITY APPLN. INFO.:			JP 1999-207957	A	19990722
			JP 2000-80734	A	20000322
			US 2000-621740	A3	20000721
			US 2002-224377	A3	20020821

OTHER SOURCE(S): MARPAT 136:12632

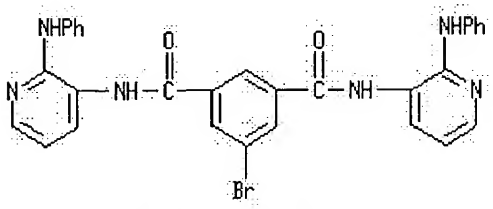
AB The invention relates to new heterocyclic compds., suited for use in making an electroluminescent device, represented by L-(A)m [A = heterocyclic group having ≥2 arom. hetero ring condensed; m = integer ≥ 2; L = bonding group].

IT **350025-83-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(in prepn. of new heterocyclic compd. for electroluminescent device)

RN 350025-83-1 HCAPLUS

h eb c g cg b cg eb

CN 1,3-Benzenedicarboxamide, 5-bromo-N,N'-bis[2-(phenylamino)-3-pyridinyl]- (9CI) (CA INDEX NAME)



L12 ANSWER 45 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Related

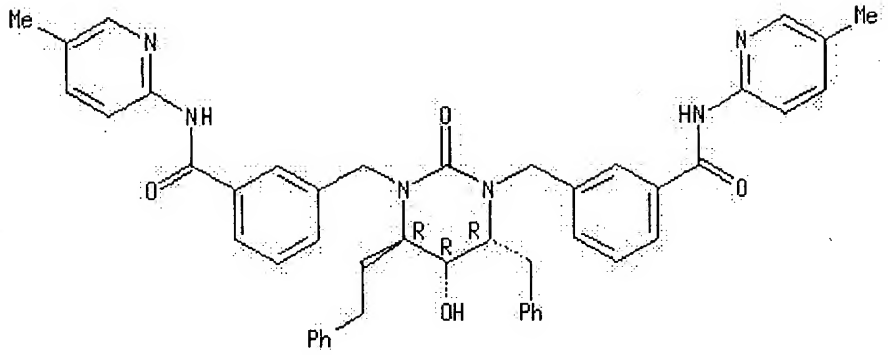
ACCESSION NUMBER: 2001:845796 HCAPLUS
DOCUMENT NUMBER: 136:79273
TITLE: A quantitative structure-activity relationship study on some HIV-1 protease inhibitors using molecular connectivity index
AUTHOR(S): Gayathri, P.; Pande, V.; Sivakumar, R.; Gupta, S. P.
CORPORATE SOURCE: Department of Chemistry, Birla Institute of Technology and Science, Pilani, 333 031, India
SOURCE: Bioorganic & Medicinal Chemistry (2001), 9(11), 3059-3063
CODEN: BMECEP; ISSN: 0968-0896
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A quant. structure-activity relation (QSAR) study has been made on two different series of tetrahydropyrimidinones acting as HIV-1 protease inhibitors. A structural parameter, the first order valence mol. connectivity index (1χv), has been used to account for the variation in the activity. The protease inhibition activity as well as the antiviral potency of the compds. are significantly correlated with 1χv of P2/P2' substituents attached to the two nitrogens N1 and N3, suggesting that substituents contg. less electroneg. and more satd. atoms, meaning thereby the less polar or more hydrophobic substituents, will be more advantageous. Further, if P2 and P2' are dissimilar, the former is more effective than the latter. This difference is attributed to a conformational change in the enzyme that may be more favorable to P2 binding than to P2' binding.

IT **219941-25-0**
RL: PAC (Pharmacological activity); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(QSAR study on HIV-1 protease inhibitors using mol. connectivity index)

RN 219941-25-0 HCAPLUS
CN Benzamide, 3,3'-[[(4R,5R,6R)-dihydro-5-hydroxy-2-oxo-4-(2-phenylethyl)-6-(phenylmethyl)-1,3(2H,4H)-pyrimidinediyl]bis(methylene)]bis[N-(5-methyl-2-pyridinyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

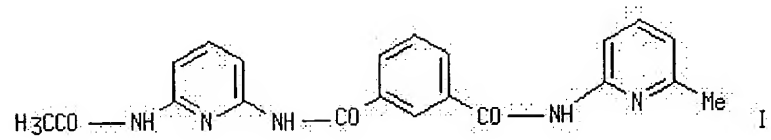


REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 46 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 2001:779567 HCAPLUS
DOCUMENT NUMBER: 136:151062
TITLE: Unsymmetrical tris-amide receptors for efficient recognition of N-acetylglycine in chloroform
AUTHOR(S): Goswami, Shyamaprosad; Mukherjee, Reshmi
CORPORATE SOURCE: Department of Chemistry, Bengal Engineering College (Deemed University), Howrah, 711 103, India
SOURCE: Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry (2001), 40B(10), 960-964
CODEN: IJSBDB; ISSN: 0376-4699
PUBLISHER: National Institute of Science Communication
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 136:151062
GI



AB A series of receptors have been designed and synthesized for recognition of sparingly sol. N-acetylglycine. Studies show that the receptor I is most efficient to bind N-acetylglycine. Binding was accomplished following a three-point hydrogen bonding strategy for carboxyl group with cooperative hydrogen bonding for acetamido group to bind guest substrate in its non-ionic form.

IT **394222-48-1P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(prepn. of pyridine amide-benzene based synthetic receptors for recognition of N-acetylglycine in chloroform)

RN 394222-48-1 HCAPLUS
CN Glycine, N-acetyl-, compd. with N-[[6-[(2,2-dimethyl-1-oxopropyl)amino]-2-pyridinyl]methyl]-N'-(6-methyl-2-pyridinyl)-1,3-benzenedicarboxamide (1:1) (9CI) (CA INDEX NAME)

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CRN 394222-46-9

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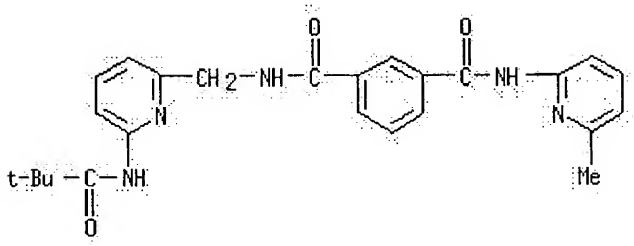
CMF C25 H27 N5 O3



CM 2

CRN 543-24-8
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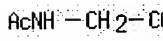


REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 47 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Check References

ACCESSION NUMBER: 2001:762969 HCAPLUS
DOCUMENT NUMBER: 135:303779
TITLE: Preparation of (hetero)arylcarboxamides as inhibitors of microsomal triglyceride transfer protein (MTP) and of apolipoprotein B (apo B) secretion.
INVENTOR(S): Damon, Robert E., II
PATENT ASSIGNEE(S): Novartis A.-G., Switz.; Novartis-Erfindungen Verwaltungsgesellschaft m.b.H.
SOURCE: PCT Int. Appl., 77 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001077077	A1	20011018	WO 2001-EP4052	20010409

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: US 2000-545620 A 20000410
OTHER SOURCE(S): MARPAT 135:303779

AB R1LCONHL1VAWZ (R1 = aryl, cycloalkyl, heterocyclyl, aralkoxy, aralkylthio; L, L1 = arylene, heteroarylene; V, W = O, S, SO, SO2, NR, bond; R = H, alkyl, aralkyl; Z = aryl, heteroaryl, heteroarylalkyl, etc.; A = alkylene; with provisos), were prepd. Thus, 6-methyl-4'-trifluoromethyl-1,1'-biphenyl-2-carboxylic acid (prepn. given), 1-hydroxy-7-azabenzotriazole,

h eb c g cg b cg eb

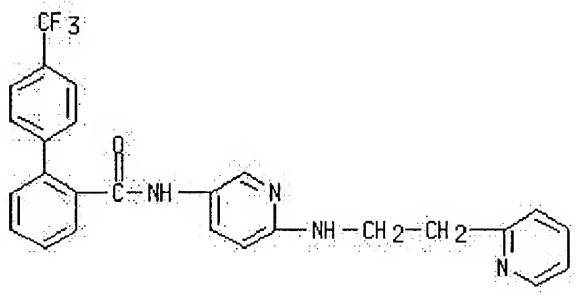
and EDCI were stirred 1 h in DMF; N1-[2-(2-pyridinyl)ethyl]-1,4-benzenediamine (prepn. given) in DMF was added followed by stirring for 16 h to give 6-methyl-N-[4-[[2-(2-pyridinyl)ethyl]amino]phenyl]-4'-(trifluoromethyl)-[1,1'-biphenyl]-2-carboxamide. The latter at 5 mg/kg orally in rats lowered both plasma triglycerides and cholesterol.

IT **366488-08-6P**

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of (hetero)arylcarboxamides as inhibitors of microsomal triglyceride transfer protein (MTP) and of apolipoprotein B (apo B) secretion)

RN 366488-08-6 HCAPLUS

CN [1,1'-Biphenyl]-2-carboxamide, N-[6-[[2-(2-pyridinyl)ethyl]amino]-3-pyridinyl]-4'-(trifluoromethyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 48 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 2001:693264 HCAPLUS
DOCUMENT NUMBER: 135:257269
TITLE: Preparation of N-heterocyclyl amide compounds as 5-HT antagonists
INVENTOR(S): Yamada, Akira; Tomishima, Masaki; Hayashida, Hisashi; Imanishi, Masashi; Spears, Glen W.; Ito, Kiyotaka; Takahashi, Fumie; Miyake, Hiroshi
PATENT ASSIGNEE(S): Fujisawa Pharmaceutical Co., Ltd., Japan
SOURCE: PCT Int. Appl., 239 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001068585	A1	20010920	WO 2001-JP1993	20010313
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
AU 2001041128	A5	20010924	AU 2001-41128	20010313

h eb c g cg b cg eb

EP 1264820 A1 20021211 EP 2001-912338 20010313
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR
US 2004087798 A1 20040506 US 2002-221554 20021227
PRIORITY APPLN. INFO.: JP 2000-70127 A 20000314
JP 2000-305947 A 20001005
WO 2001-JP1993 W 20010313

OTHER SOURCE(S): CASREACT 135:257269; MARPAT 135:257269

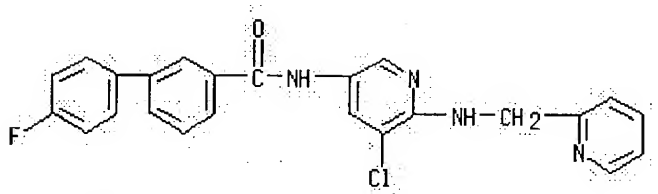
AB Amides compds. represented by the general formula R1-A-X-NHCO-Y-R2 [wherein R1 is an optionally substituted heterocyclic group or optionally substituted phenyl; R2 is optionally substituted fused Ph, optionally substituted Ph, or optionally substituted thienyl; A is a group represented by the formula -(CH2)t-(O)m- or -(CR3R4)pNR5(CO)n- (wherein R3 and R4 each is hydrogen or R3 and R4 in combination form imino; R5 is hydrogen or lower alkyl; t is 0, 1, or 2; and p, m, and n each is 0 or 1); X is optionally substituted phenylene or an optionally substituted, divalent, nitrogenous heterocyclic group; and Y is a bond, lower alkylene, or lower alkenylene] and salts thereof are prepd. Theses amides include phenylacetamide, cinnamides, 1H-indole-7-carboxamides, 3-(2-pyridyl)-2-propenamides, 5-phenyl-2-thiophenecarboxamides, 9H-carbazolecarboxamides, 3-phenyl-2-propenamides, 9H-fluorene-1-carboxamides, 2,3-dihydrobenz[b]oxepine-4-carboxamides, 1H-benzo[b]thiepin-4-carboxamides, and 3-(1H-indol-3-yl)-2-propenamides. They are antagonists of 5-hydroxytryptamine (5-HT), in particular 5-HT2c, and are useful for the treatment of 5-HT-mediated diseases such as (1) central nervous system disorders in including anxiety, depression, obsessive-compulsive neurosis, migraine headache, anorexia, Alzheimer's disease, sleep disorder, over-eating, and panic, (2) withdrawal symptom caused by cocaine, ethanol, nicotine, and benzodiazepine, (3) schizophrenia, (4) spinal cord injury, and /or (5) head injury such as hydrocephalus. Thus, SOCl2 was added to a soln. of (E)-4-phenyl-3-butenoic acid in benzene, heated under reflux for 1 h, and cooled, followed by adding 3-(imidazol-1-yl)aniline and Et3N, and the resulting mixt. was stirred at room temp. for 1 h to give (3E)-N-[3-(imidazol-1-yl)phenyl]-4-phenyl-3-butenamide (I). I in vitro inhibited by 82% the binding of [3H]mesulergine to 5-HT2c receptor which was prepd. from rat frontal lobe cortex.

IT **361551-35-1P**

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of N-heterocyclyl amide compds. as 5-HT antagonists for treatment of 5-HT-mediated diseases such as central nervous system disorders, drug withdrawal symptom, schizophrenia, spinal code injury, and head injury)

RN 361551-35-1 HCAPLUS

CN [1,1'-Biphenyl]-3-carboxamide, N-[5-chloro-6-[(2-pyridinylmethyl)amino]-3-pyridinyl]-4'-fluoro- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 49 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

h eb c g cg b cg eb

Full Text | Citing References

ACCESSION NUMBER: 2001:661392 HCAPLUS
DOCUMENT NUMBER: 135:226888
TITLE: Preparation of pyridyl benzamides and related compounds as Factor Xa inhibitors.
INVENTOR(S): Zhu, Bing-yan; Zhang, Penglie; Wang, Lingyan; Huang, Wenrong; Goldman, Erick; Li, Wenhao; Zuckett, Jingmei; Song, Yonghong; Scarborough, Robert
PATENT ASSIGNEE(S): Cor Therapeutics, Inc., USA
SOURCE: PCT Int. Appl., 322 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 6
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001064643	A2	20010907	WO 2001-US6255	20010228
WO 2001064643	A3	20020404		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
EP 1259485	A2	20021127	EP 2001-918257	20010228
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				

PRIORITY APPLN. INFO.:

US 2000-185746P	P	20000229
US 2000-663420	A	20000915
WO 2001-US6255	W	20010228

OTHER SOURCE(S): MARPAT 135:226888

AB AQDEGJX [A = alkyl, cycloalkyl, NR1R2, NR1R2C(:NR3), (substituted) Ph, naphthyl, heterocyclyl, etc.; R1-R3 = H, OR5, NR5R6, alkyl, alkenyl, etc.; R1R2 or R2R3 = atoms to form (substituted) cycloalkyl, heterocyclyl; R5, R6 = H, alkyl, alkenyl, alkynyl, cycloalkyl, (substituted) alkylphenyl, alkylnaphthyl; R5R6 = atoms to form a 3-8 membered (substituted) ring; Q = bond, CH2, CO, O, S, SO, SO2, NR7, SO2NR7, etc.; R7 = H, alkyl, alkenyl, alkynyl, cycloalkyl, alkylcycloalkyl, (substituted) alkylphenyl, alkylnaphthyl; D = bond, (substituted) Ph, naphthyl, mono- or bicyclic heterocyclyl; E = bond, alkyl, O, S, SO, SO2, alkylcarbonyl, etc.; G = (substituted) alkenyl, cycloalkenyl, phenylene, 3-8 membered (fused) (arom.) heterocyclyl; J = bond, NR9CO, O, S, SO, SO2, CH2, NR9SO2, etc.; X = (substituted) Ph, naphthyl, (fused) heteroaryl], were prepd. as antithrombotics (no data). Thus, N-(5-bromo-2-pyridinyl)-2-aminophenylcarboxamide (prepn. given), 4-cyanobenzoyl chloride, and pyridine were stirred overnight in CH2Cl2 to give 70% N-(5-bromo-2-pyridinyl)-[2-(4-cyanophenylcarbonyl)amino]phenylcarboxamide. The latter in MeOH at 0° was satd. with HCl and stirred overnight followed by solvent evapn. The residue was refluxed 2 h with NH4OAc in MeOH to give 70% N-(5-bromo-2-pyridinyl)-[2-(4-amidinophenylcarbonyl)amino]phenylcarboxamide.

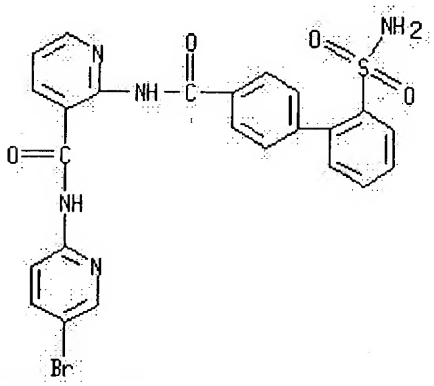
IT **330939-74-7P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);

h eb c g cg b cg eb

BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of pyridyl benzamides and related compds. as Factor Xa inhibitors)

RN 330939-74-7 HCAPLUS

CN 3-Pyridinecarboxamide, 2-[[[2'-(aminosulfonyl)[1,1'-biphenyl]-4-yl]carbonyl]amino]-N-(5-bromo-2-pyridinyl)- (9CI) (CA INDEX NAME)



L12 ANSWER 50 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 2001:661391 HCAPLUS
DOCUMENT NUMBER: 135:210946
TITLE: Preparation of pyridylamides as Factor Xa inhibitors.
INVENTOR(S): Zhu, Bing-yan; Zhang, Penglie; Wang, Lingyan; Huang, Wenrong; Goldman, Erick; Li, Wenhao; Zuckett, Jingmei; Song, Yonghong; Scarborough, Robert
PATENT ASSIGNEE(S): Cor Therapeutics, Inc., USA
SOURCE: PCT Int. Appl., 306 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 6
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001064642	A2	20010907	WO 2001-US6247	20010228
WO 2001064642	A3	20020502		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: US 2000-185746P P 20000229
US 2000-663420 A 20000915

OTHER SOURCE(S): MARPAT 135:210946

AB AQDEGJX [A = alkyl, cycloalkyl, NR1R2, NR1R1C(:NR3), (substituted) Ph, naphthyl, mono- or bicyclic heterocyclyl, etc.; R1-R3 = H, alkyl, alkenyl, alkynyl, cycloalkyl, (alkyl)aryl, (alkyl)heteroaryl, etc.; R1R2 or R2R3 = atoms to form a 3-8 membered (substituted) (heterocyclic) ring; Q = bond, CH2, CO, O, NR7, etc.; R7 = H, alkyl, (alkyl)aryl, (alkyl)heteroaryl,

h eb c g cg b cg eb

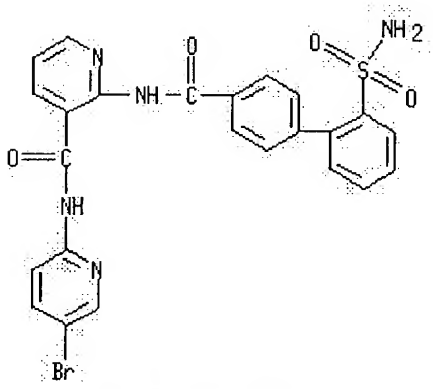
etc.; D = bond, (substituted) Ph, naphthyl, mono- or bicyclic heterocyclyl; E = bond, alkyl, S, SO, SO2, alkoxy, etc.; G = (substituted) alkenyl, cycloalkenyl, phenylene, heterocyclyl, fused cyclic system; J = bond, NR9CO, O, S, SO, SO2, SO2NR9, CH2, NR9, etc.; R9 = H, alkyl, (alkyl)aryl, etc.; X = (substituted) Ph, naphthyl, heteroaryl, fused bicyclyl], were prepd. as antithrombotics (no data). Thus, N-(5-bromo-2-pyridinyl) 2-aminophenylcarboxamide (prepn. given), 4-[(2-tert-butylaminosulfonyl)phenyl]benzoyl chloride, and pyridine were stirred overnight in CH2Cl2 to give 85% N-(5-bromo-2-pyridinyl)-[2-4-[(2-aminosulfonyl)phenyl]phenylcarbonylamino]phenylcarboxamide.

IT **330939-74-7P**

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of pyridylamides as Factor Xa inhibitors)

RN 330939-74-7 HCAPLUS

CN 3-Pyridinecarboxamide, 2-[[[2'-(aminosulfonyl)[1,1'-biphenyl]-4-yl]carbonyl]amino]-N-(5-bromo-2-pyridinyl)- (9CI) (CA INDEX NAME)



L12 ANSWER 51 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 2001:606591 HCAPLUS
DOCUMENT NUMBER: 136:369580
TITLE: Design and synthesis of tweezers-like artificial receptor of aromatic heterocycles based on multiple hydrogen-bonding sites
AUTHOR(S): Zhao, Zhiming; Mu, Qiming; Hu, Rong; Yang, Zuxing; Chen, Shuhau
CORPORATE SOURCE: Faculty of Chemistry, Sichuan University, Chengdu, 610064, Peop. Rep. China
SOURCE: Sichuan Daxue Xuebao, Ziran Kexueban (2001), 38(3), 402-406
CODEN: SCTHAO; ISSN: 0490-6756
PUBLISHER: Sichuan Daxue Xuebao Bianjibu
DOCUMENT TYPE: Journal
LANGUAGE: Chinese
OTHER SOURCE(S): CASREACT 136:369580

AB Eight mol. tweezers 2,6-dibenzamidopyridine, 2,6-di(4-ethoxybenzamido)pyridine, 2,2'-di(pyridine-2-aminocarbonyl)diphenyl, 1,3-di(phenoxyacetamido)pyridine, 1,2-di(phenoxyacetamido)pyridine, 1,3-di(6-benzamidopyridine-2-aminocarbonyl)benzene, 1,3-di[6-(4-nitrobenzamido)pyridine-2-aminocarbonyl]benzeene, and 1,3-di(6-benzamidopyridine-2-aminocarbonyl)pyridine were designed and synthesized by acylation. The structures of these receptors were identified by MS,

h eb c g cg b cg eb

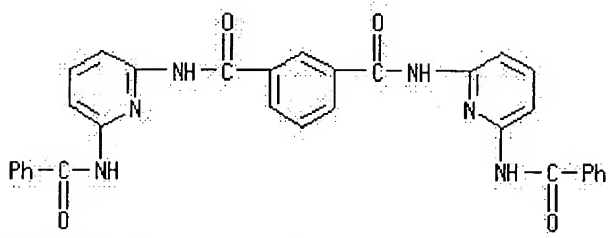
1HNMR, and IR spectra.

IT **425377-08-8P**

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (synthesis of tweezers-like artificial receptor of arom. heterocycles based on multiple hydrogen-bonding sites)

RN 425377-08-8 HCAPLUS

CN 1,3-Benzenedicarboxamide, N,N'-bis[6-(benzoylamino)-2-pyridinyl]- (9CI) (CA INDEX NAME)



L12 ANSWER 52 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Linked References

ACCESSION NUMBER: 2001:564991 HCAPLUS
DOCUMENT NUMBER: 135:137828
TITLE: Functional monomers for molecular recognition and catalysis
INVENTOR(S): Sellergren, Boerje; Hall, Andrew; Chenon, Karine; Karmalkar, Rohini
PATENT ASSIGNEE(S): Mip Technologies AB, Swed.
SOURCE: PCT Int. Appl., 59 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001055095	A1	20010802	WO 2001-SE137	20010125
W: AE, AG, AL, AM, AT, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, CZ, DE, DE, DK, DK, DM, DZ, EE, EE, ES, FI, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
EP 1250315	A1	20021023	EP 2001-902904	20010125
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
JP 2003520843	T2	20030708	JP 2001-555037	20010125
US 2003166798	A1	20030904	US 2002-169799	20021125
PRIORITY APPLN. INFO.:			SE 2000-295 A	20000128
			SE 2000-389 A	20000128
			WO 2001-SE137 W	20010125

OTHER SOURCE(S): MARPAT 135:137828

AB The present invention refers to new classes of polymerizable monomers, to molecularly imprinted polymers obtainable by polymn. of at least one of

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the monomers and a crosslinking monomer in the presence of a template mol. The obtained polymers may be used for sepn. of enantiomers, diastereomers of the template mol., and also for sepn. of the template mol. or template mol. analogs from structurally related compds. The monomers can be formamidines, chiral amidines, vinyl- methacryloyl or acryloyl-based alkyl or aryldiamines, receptor analog monomers, etc.

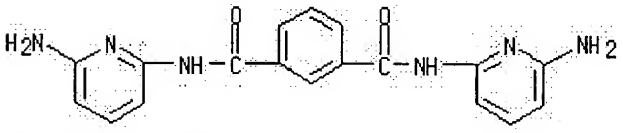
IT **112817-57-9P**

RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)

(functional monomers for mol. recognition and catalysis)

RN 112817-57-9 HCAPLUS

CN 1,3-Benzenedicarboxamide, N,N'-bis(6-amino-2-pyridinyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 53 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | More References

ACCESSION NUMBER: 2001:545674 HCAPLUS

DOCUMENT NUMBER: 135:137516

TITLE: Synthesis of heteroarylbenzamides and analogs used for inhibiting protein kinases

INVENTOR(S): Bender, Steven Lee; Bhumralkar, Dilip; Collins, Michael Raymond; Cripps, Stephan James; Deal, Judith Gail; Nambu, Mitchell David; Palmer, Cynthia Louise; Peng, Zhengwei; Varney, Michael David; Jia, Lei

PATENT ASSIGNEE(S): Agouron Pharmaceuticals, Inc., USA

SOURCE: PCT Int. Appl., 237 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001053274	A1	20010726	WO 2001-US1723	20010119
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
US 2002103203	A1	20020801	US 2001-764306	20010119
US 6635641	B2	20031021		
EP 1252146	A1	20021030	EP 2001-906592	20010119
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
BR 2001008025	A	20021105	BR 2001-8025	20010119

h eb c g cg b cg eb

JP 2003529558	T2	20031007	JP 2001-553276		20010119
US 2004092747	A1	20040513	US 2003-621979		20030717
PRIORITY APPLN. INFO.:			US 2000-177059P	P	20000121
			US 2001-764306	A3	20010119
			WO 2001-US1723	W	20010119

OTHER SOURCE(S): MARPAT 135:137516
GI

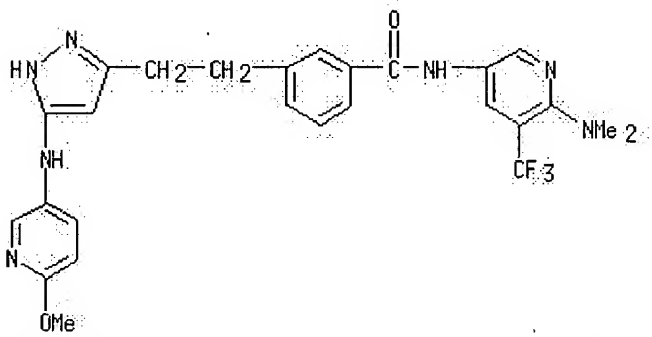
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Title compds. I [Z = CH, NH; Q = moiety such that ring A is (un)substituted mono- or bicyclic heteroaryl which has at least 2 carbon atoms in the heteroaryl ring system; X = CH2, O, S, NH; Y = CH2, O, S, provided at least one of X and Y = CH2 or X and Y form a cyclopropyl ring; R2-3 = H, Me, halo, CF3, CN; R4 = CONHR5, NHCOR6; where R5 = (un)substituted aryl, heteroaryl, cycloalkyl, etc.; R6 = (un)substituted aryl, heteroaryl, cycloalkyl, etc] are prepd. Examples include synthetic procedures for over 150 compds., 11 biol. assays and 3 sample formulations. For instance, 3-mercaptobenzoic acid was treated with α-chloro-N-methoxy-N-methylacetamide followed by carbodiimide coupling to 2-methyl-6-aminoquinoline to give II. II was converted to a β-thiono-ketone with thioacetanilide/n-BuLi followed by treatment with hydrazine to give pyrazole III. III gave 85% inhibition of an lck protein tyrosine kinase at 5 μM and had Ki = 2.21 nM for VEGF-R2Δ50. Treatment of cancer as well as other disease states assocd. with unwanted angiogenesis and/or cellular proliferation, such as diabetic retinopathy, neovascular glaucoma, rheumatoid arthritis, and psoriasis are claimed uses of the invention.

IT **351320-27-9P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(synthesis of heteroarylbenzamides used for inhibiting protein kinases)

RN 351320-27-9 HCAPLUS

CN Benzamide, N-[6-(dimethylamino)-5-(trifluoromethyl)-3-pyridinyl]-3-[2-[5-[(6-methoxy-3-pyridinyl)amino]-1H-pyrazol-3-yl]ethyl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 54 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

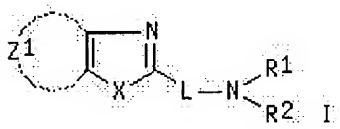
Full Text | (1) References

h eb c g cg b cg eb

ACCESSION NUMBER: 2001:517740 HCAPLUS
DOCUMENT NUMBER: 135:114270
TITLE: Novel condensed hetero ring compound and electroluminescent material
INVENTOR(S): Ise, Toshihiro; Okada, Hisashi
PATENT ASSIGNEE(S): Fuji Photo Film Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 36 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
JP 2001192653	A2	20010717	JP 2000-89632		20000328
US 6620529	B1	20030916	US 2000-697157		20001027
US 2004146745	A1	20040729	US 2003-625539		20030724
PRIORITY APPLN. INFO.:			JP 1999-305733	A	19991027
			JP 2000-62472	A	20000307
			JP 2000-89632	A	20000328
			US 2000-697157	A3	20001027

GI

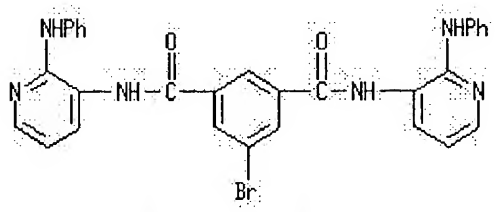


I

AB The invention refers to a novel condensed hetero ring compd. I [R1,2 = H, aliph. hydrocarbon, aryl or hetero ring; Z1 = atoms need to construct a heterocyclic; L = bridging functional group; X = O, S, Se, Trace element or N-R; R = H, aliph. hydrocarbon, aryl or heterocyclic].

IT **350025-83-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(novel condensed hetero ring compd. and electroluminescent material)

RN 350025-83-1 HCAPLUS
CN 1,3-Benzenedicarboxamide, 5-bromo-N,N'-bis[2-(phenylamino)-3-pyridinyl]- (9CI) (CA INDEX NAME)



L12 ANSWER 55 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 2001:361910 HCAPLUS
DOCUMENT NUMBER: 135:122741
TITLE: Synthesis based on affinity separation (SAS): separation of products having barbituric acid tag from untagged compounds by using hydrogen bond interaction

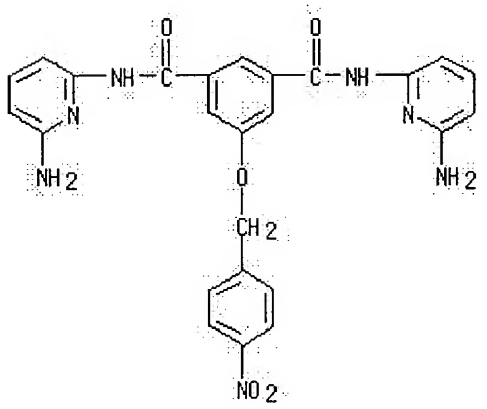
h eb c g cg b cg eb

AUTHOR(S): Zhang, San-Qi; Fukase, Koichi; Izumi, Minoru; Fukase, Yoshiyuki; Kusumoto, Shoichi
CORPORATE SOURCE: Department of Chemistry, Graduate School of Science, Osaka University, Osaka, 560-0043, Japan
SOURCE: Synlett (2001), (5), 590-596
CODEN: SYNLES; ISSN: 0936-5214
PUBLISHER: Georg Thieme Verlag
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 135:122741

AB A new method is described for affinity purifn. of synthetic compds. based on mol. recognition between bis(2,6-diaminopyridine)amide of isophthalic acid and a barbituric acid deriv. The desired compds. possessing the barbituric acid deriv. as a tag were readily isolated from the reaction mixt. by the following procedure. After each reaction cycle, the reaction mixt. was applied to the polystyrene column possessing bis(2,6-diaminopyridine)amide of isophthalic acid as an artificial receptor. The compd. possessing the barbituric acid tag was selectively adsorbed on the column, whereas other impurities without the tag such as excess reagents and byproducts were washed off. Subsequent desorption with CH2Cl2-MeOH (1:1) afforded the desired compd. with high purity. This new strategy was applied to the synthesis of a heterocycle, peptides, and oligosaccharides.

IT **350671-22-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of peptides or oligosaccharides using barbituric acid tags for affinity chromatog. sepn. of products)

RN 350671-22-6 HCAPLUS
CN 1,3-Benzenedicarboxamide, N,N'-bis(6-amino-2-pyridinyl)-5-[(4-nitrophenyl)methoxy]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 56 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 2001:208239 HCAPLUS
DOCUMENT NUMBER: 134:252153
TITLE: Preparation of benzamides as inhibitors of factor Xa
INVENTOR(S): Zhu, Bing-yan; Zhang, Penglie; Wang, Lingyan; Huang, Wenrong; Goldman, Eric; Li, Wenhao; Zuckett, Jingmei; Song, Yonghong; Scarborough, Robert
PATENT ASSIGNEE(S): Cor Therapeutics, Inc., USA

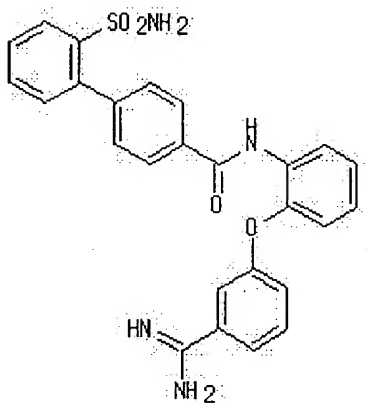
h eb c g cg b cg eb

SOURCE: PCT Int. Appl., 224 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 6
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001019788	A2	20010322	WO 2000-US25196	20000915
WO 2001019788	A3	20010809		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
AU 2000074867	A5	20010417	AU 2000-74867	20000915
EP 1216228	A2	20020626	EP 2000-963452	20000915
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL				
BR 2000014076	A	20021015	BR 2000-14076	20000915
JP 2003509406	T2	20030311	JP 2001-523368	20000915
NO 2002001229	A	20020521	NO 2002-1229	20020312

PRIORITY APPLN. INFO.:	US 1999-154332P	P	19990917
	US 2000-185746P	P	20000229
	WO 2000-US25196	W	20000915

OTHER SOURCE(S): MARPAT 134:252153
GI



I

AB The title compds. AQDEGJX [A = alkyl, cycloalkyl, (un)substituted Ph, etc.; Q = a direct link, CH2, CO, etc.; D = a direct link, (un)substituted Ph, naphthyl, etc.; E = a direct link, O, alkyl, etc.; G = alkenylene, cycloalkenylene, phenylene, etc.; J = a direct link, O, S, etc.; X = a (un)substituted Ph, naphthyl, heteroaryl, etc.] having activity against mammalian factor Xa (no data), and useful in vitro or in vivo for preventing or treating coagulation disorders, were prepd. E.g., a 4-step synthesis of the benzamide I was given.

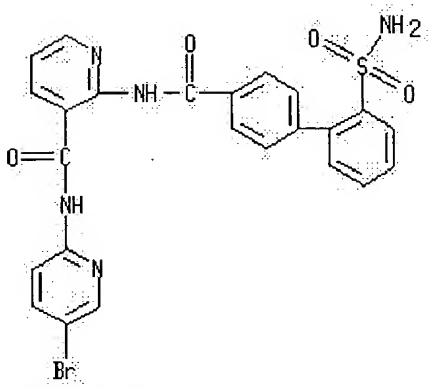
IT **330939-74-7P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);

h eb c g cg b cg eb

BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of benzamides as inhibitors of factor Xa)

RN 330939-74-7 HCAPLUS

CN 3-Pyridinecarboxamide, 2-[[[2'-(aminosulfonyl)[1,1'-biphenyl]-4-yl]carbonyl]amino]-N-(5-bromo-2-pyridinyl)- (9CI) (CA INDEX NAME)



L12 ANSWER 57 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 2001:139754 HCAPLUS
DOCUMENT NUMBER: 134:340873
TITLE: Effect of an Internal Anthranilamide Turn Unit on the Structure and Conformational Stability of Helically Biased Intramolecularly Hydrogen-Bonded Dendrons
AUTHOR(S): Huang, Baohua; Parquette, Jon R.
CORPORATE SOURCE: Department of Chemistry, The Ohio State University, Columbus, OH, 43210, USA
SOURCE: Journal of the American Chemical Society (2001), 123(11), 2689-2690
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB We have described dendrons that exhibit a helical secondary structure that occurs over three generational levels. The preliminary evidence described in this paper suggests that mol. packing plays an important role in stabilizing secondary structure in dendrimeric systems.

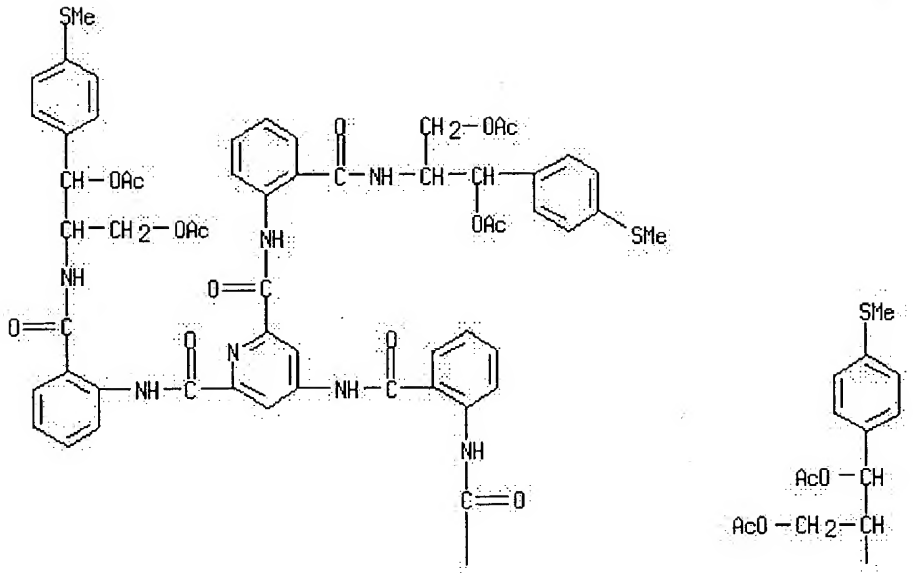
IT **337955-55-2**
RL: PRP (Properties)
(effect of internal anthranilamide turn unit on structure and conformational stability of helically biased intramolecularly hydrogen-bonded dendrons)

RN 337955-55-2 HCAPLUS

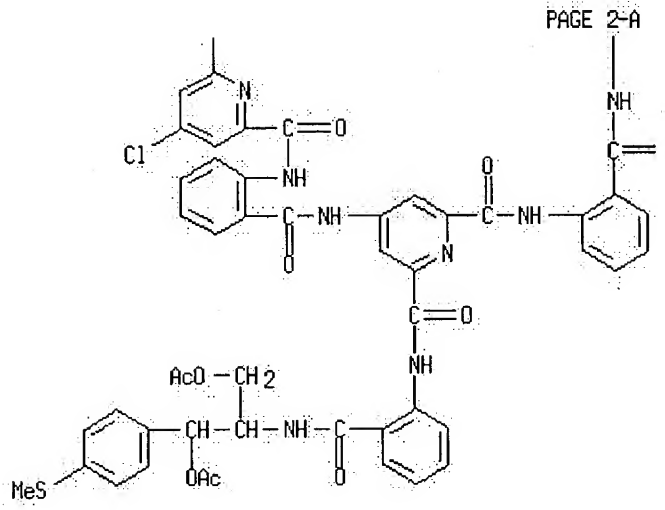
CN 2,6-Pyridinedicarboxamide, N,N'-bis[2-[[[2,6-bis[[[2-[[[2-(acetyloxy)-1-[(acetyloxy)methyl]-2-[4-(methylthio)phenyl]ethyl]amino]carbonyl]phenyl]amino]carbonyl]-4-pyridinyl]amino]carbonyl]phenyl]-4-chloro- (9CI) (CA INDEX NAME)

h eb c g cg b cg eb

PAGE 1-A



PAGE 2-A



PAGE 2-B

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REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

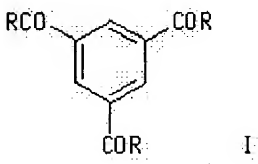
L12 ANSWER 58 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Cited References

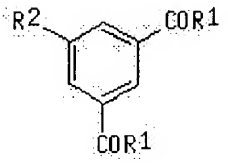
ACCESSION NUMBER: 2001:120738 HCAPLUS
DOCUMENT NUMBER: 134:326418
TITLE: Molecular recognition of carbohydrates by artificial receptors: systematic studies towards recognition motifs for carbohydrates
AUTHOR(S): Mazik, Monika; Sicking,' Willi
CORPORATE SOURCE: Institut fur Organische Chemie der Universitat Essen,

h eb c g cg b cg eb

Essen, 45117, Germany
SOURCE: Chemistry--A European Journal (2001), 7(3), 664-670
CODEN: CEUJED; ISSN: 0947-6539
PUBLISHER: Wiley-VCH Verlag GmbH
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I



II

AB Several acyclic artificial receptors, benzene derivs. I (R = 7-methyl-1,8-naphthyridin-2-ylamino, 6-methyl-2-pyridinyloxy, 3,5-dimethylphenylamino) and II (R1 = 7-methyl-1,8-naphthyridin-2-ylamino, R2 = H; R1 = 6-methyl-2-pyridinylamino, R2 = 6,7-dimethoxy-2-oxo-2H-chromen-4-ylmethoxy), were synthesized as artificial receptors for the binding of an octyl β-D-glucopyranoside mol. These artificial receptors having uncharged hydrogen-bonding sites were used in a systematic study towards the evaluation of recognition motifs for carbohydrates. A novel effective, acyclic hydrogen-bonding receptor possessing naphthyridine - amide moieties as heterocyclic recognition units has been developed.

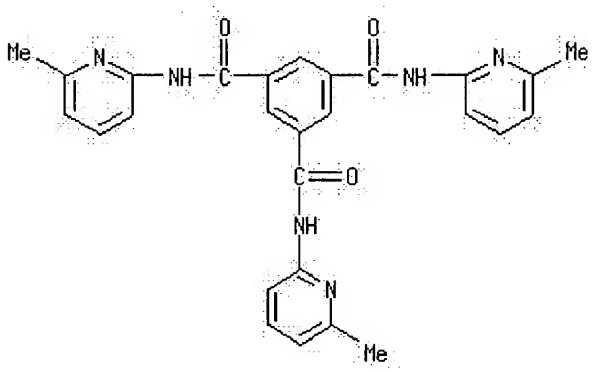
IT **264626-71-3**
RL: FMU (Formation, unclassified); PRP (Properties); FORM (Formation, nonpreparative)
(formation of a 1:1 complex of a heterocyclic artificial receptor with a glucoside mol.)

RN 264626-71-3 HCAPLUS

CN β-D-Glucopyranoside, octyl, compd. with N,N',N''-tris(6-methyl-2-pyridinyl)-1,3,5-benzenetricarboxamide (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 164174-81-6
CMF C27 H24 N6 O3



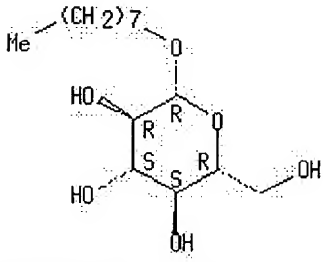
CM 2

CRN 29836-26-8

h eb c g cg b cg eb

CMF C14 H28 O6

Absolute stereochemistry. Rotation (-).



REFERENCE COUNT: 39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 59 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | More References

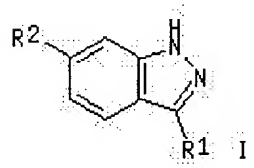
ACCESSION NUMBER: 2001:31473 HCAPLUS
DOCUMENT NUMBER: 134:100864
TITLE: Indazole compounds and pharmaceutical compositions for inhibiting protein kinases, and methods for their use
INVENTOR(S): Kania, Robert Steven; Bender, Steven Lee; Borchardt, Allen J.; Braganza, John F.; Cripps, Stephan James; Hua, Ye; Johnson, Michael David; Johnson, Theodore Otto, Jr.; Luu, Hiep The; Palmer, Cynthia Louise; Reich, Siegfried Heinz; Tempczyk-russell, Anna Maria; Teng, Min; Thomas, Christine; Varney, Michael David; Wallace, Michael Brennan
PATENT ASSIGNEE(S): Agouron Pharmaceuticals, Inc., USA
SOURCE: PCT Int. Appl., 439 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001002369	A2	20010111	WO 2000-US18263	20000630
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
BR 2000012352	A	20020514	BR 2000-12352	20000630
EP 1218348	A2	20020703	EP 2000-943375	20000630
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL				
JP 2003503481	T2	20030128	JP 2001-507809	20000630
NZ 516676	A	20030926	NZ 2000-516676	20000630
US 6531491	B1	20030311	US 2001-983786	20011025
US 6534524	B1	20030318	US 2001-983783	20011025
NO 2001005797	A	20020301	NO 2001-5797	20011128
ZA 2001010061	A	20030206	ZA 2001-10061	20011206

h eb c g cg b cg eb

BG 106380	A	20020930	BG 2002-106380		20020201
US 2004171634	A1	20040902	US 2003-326755		20030213
PRIORITY APPLN. INFO.:			US 1999-142130P	P	19990702
			US 2000-609335	B3	20000630
			WO 2000-US18263	W	20000630
			US 2001-983786	A3	20011025

OTHER SOURCE(S): MARPAT 134:100864
GI



I

AB Indazole compds. I [R1 = substituted or unsubstituted aryl or heteroaryl, R3CH:CH, R3N:CH; R2 = substituted or unsubstituted aryl, heteroaryl, Y-X; R3 = substituted or unsubstituted alkyl alkenyl, cycloalkyl, heterocycloalkyl, aryl, heteroaryl; Y = O, S, C(:CH2), CO, SO, SO2, alkylidene, NH, N(C1-C8 alkyl); X = substituted or unsubstituted aryl, heteroaryl, NH(alkyl), NH(cycloalkyl), NH(heterocycloalkyl), NH(aryl), NH(heteroaryl), NH(alkoxy), NH(dialkylamide)] and their pharmaceutically acceptable prodrugs, active metabolites, and salts are disclosed. The compds. modulate and/or inhibit the activity of certain protein kinases. In particular, I and pharmaceutical compns. contg. them are capable of mediating tyrosine kinase signal transduction, and thereby modulate and/or inhibit unwanted cell proliferation. The invention is also directed to the therapeutic or prophylactic use of pharmaceutical compns. contg. such compds., and to methods of treating cancer and other disease states assocd. with unwanted angiogenesis and/or cellular proliferation, such as diabetic retinopathy, neovascular glaucoma, rheumatoid arthritis, and psoriasis, by administering effective amts. of such compds. E.g., I [R1 = (E)-3,4-(MeO)2C6H3CH:CH; R2 = 4-HO-3-MeOC6H3] (II) was prepd. from 6-aminoindazole by diazotization and substitution with iodide, protection of the indazole nitrogen with 2,4,6-Me3C6H2SO2Cl, coupling of the regioisomeric mixt. with 4-(methoxymethoxy)-3-methoxybenzeneboronic acid in the presence of dichlorobis(triphenylphosphine)palladium, and deprotection of the indazole moiety and iodination at the 3-position of the indazole. Treatment of the 3-indazolyl iodide with sec-butyllithium, phenyllithium, and DMF, regioselective protection of the indazole with 2,4,6-Me3C6H2SO2Cl, olefination with 3,4-dimethoxybenzyltriphenylphosphonium bromide, deprotection of the indazole, deprotection of the methoxymethyl group, and equilibration of the double bond with iodine gave II. Biol. data on protein kinase inhibition, cell proliferation inhibition, neovascularization inhibition, and i.p. and oral bioavailability, are given.

IT **319468-88-7P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of combinatorial libraries of aryl-substituted indazole derivs. as modulators and inhibitors of protein kinases in the treatment of tumor growth, cellular proliferation, and angiogenesis)

RN 319468-88-7 HCAPLUS
CN Benzamide, 2-[[3-[(1E)-2-(2-pyridinyl)ethenyl]-1H-indazol-6-yl]thio]-N-[5-(trifluoromethyl)-2-pyridinyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

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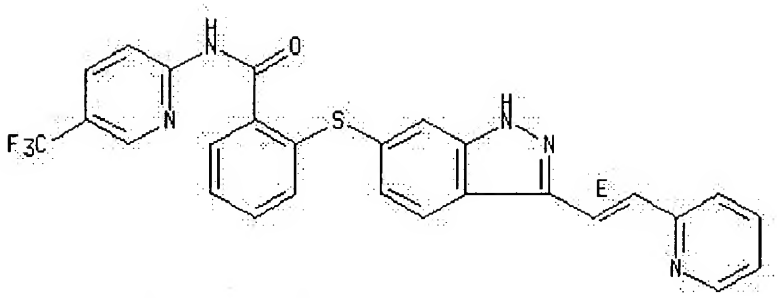


L12 ANSWER 60 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | More References

ACCESSION NUMBER: 2000:908053 HCAPLUS
DOCUMENT NUMBER: 134:207440
TITLE: Selective Binding of cis-1,3,5-Cyclohexane Tricarboxylic Acid vs Its Epimeric trans Isomer by a Tripodal Amidopyridine Receptor; Crystal Structures of the 1:1 Complexes
AUTHOR(S): Ballester, Pablo; Capo, Magdalena; Costa, Antoni; Deya, Pere M.; Gomila, Rosa; Decken, Andreas; Deslongchamps, Ghislain
CORPORATE SOURCE: Departament de Quimica, Universitat de les Illes Balears, Palma de Mallorca, 07071, Spain
SOURCE: Organic Letters (2001), 3(2), 267-270
CODEN: ORLEF7; ISSN: 1523-7060
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A tripodal tris-amidopyridine receptor forms a 1:1 complex with trans-1,3,5-cyclohexane tricarboxylic acid that is 1 order of magnitude less stable than the one formed with the corresponding cis-triacid epimer. The X-ray crystal structures of the complexes have been detd., confirming the binding geometry derived from NMR data in soln. and force-field calcns., and its geometrical features are used to explain the obsd. selectivity.

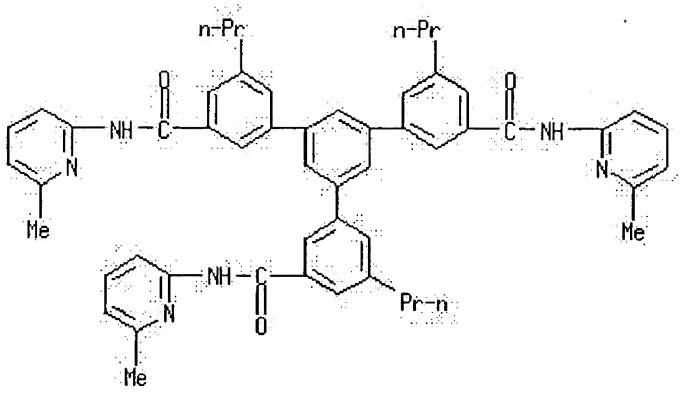
IT **329005-98-3P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (crystal structure; selective binding of cis-1,3,5-cyclohexane tricarboxylic acid vs its epimeric trans isomer by a tripodal amidopyridine receptor)

RN 329005-98-3 HCAPLUS

CN 1,3,5-Cyclohexanetricarboxylic acid, (1α,3α,5α)-, compd. with N,N'-bis(6-methyl-2-pyridinyl)-5'-[3-[[(6-methyl-2-pyridinyl)amino]carbonyl]-5-propylphenyl]-5,5''-dipropyl[1,1':3',1''-terphenyl]-3,3''-dicarboxamide (1:1) (9CI) (CA INDEX NAME)

CM 1

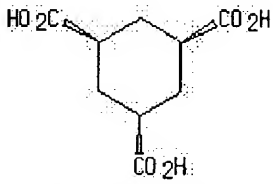
CRN 221021-04-1
CMF C54 H54 N6 O3



CM 2

CRN 16526-68-4
CMF C9 H12 O6

Relative stereochemistry.



REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 61 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | More References

ACCESSION NUMBER: 2000:814461 HCAPLUS
DOCUMENT NUMBER: 133:362707
TITLE: Preparation of pyridylethylpyridines as phosphodiesterase 4 inhibitors.
INVENTOR(S): Cote, Bernard; Friesen, Richard; Frenette, Richard; Girard, Mario; Girard, Yves; Godbout, Cedrickx; Guay, Daniel; Hamel, Pierre; Blouin, Marc; Ducharme, Yves; Prescott, Sylvie
PATENT ASSIGNEE(S): Merck Frosst Canada & Co., Can.
SOURCE: PCT Int. Appl., 155 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000068198	A2	20001116	WO 2000-CA500	20000503
WO 2000068198	A3	20010405		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

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RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

US 6200993		B1	20010313	US 2000-551040	20000417
EP 1177175		A2	20020206	EP 2000-922400	20000503
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
AU 764258		B2	20030814	AU 2000-42829	20000503
PRIORITY APPLN. INFO.:				US 1999-132532P	P 19990505
				WO 2000-CA500	W 20000503

OTHER SOURCE(S): MARPAT 133:362707

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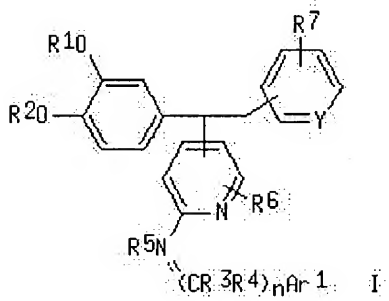

I

AB Title compds. [I; Y = N, NO; R1, R2 = H, alkyl, haloalkyl; R3, R4 = H, alkyl; R3R4 = O, atoms to form a 5-7 membered carbocyclic ring; R5 = null, H, (substituted) alkyl, alkylcarbonyl, arylcarbonyl, alkoxycarbonyl, aryloxycarbonyl, O; R3R5 = atoms to form a 5-6 membered heterocyclic ring; dotted line = optional double bond; R6, R7 = H, halo, alkyl, haloalkyl, cyano; n = 0-6], were prepd. Thus, 4-[2-[3,4-bis(difluoromethoxy)phenyl]-2-(6-bromo-3-pyridyl)ethyl]pyridine (prepn. given) was heated with PhCH2NH2 and CuI to give 72% 4-[2-[3,4-bis(difluoromethoxy)phenyl]-2-[6-(benzylamino)-3-pyridyl]ethyl]pyridine. The latter inhibited PDE 4 with IC50 = 0.75 nM.

IT **306760-86-1P**

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(prepn. of pyridylethylpyridines as phosphodiesterase 4 inhibitors)

RN 306760-86-1 HCAPLUS

CN Benzamide, N-[5-[1-[3,4-bis(difluoromethoxy)phenyl]-2-(1-oxido-4-pyridinyl)ethyl]-2-pyridinyl]-4-fluoro-N-(4-fluorobenzoyl)- (9CI) (CA INDEX NAME)

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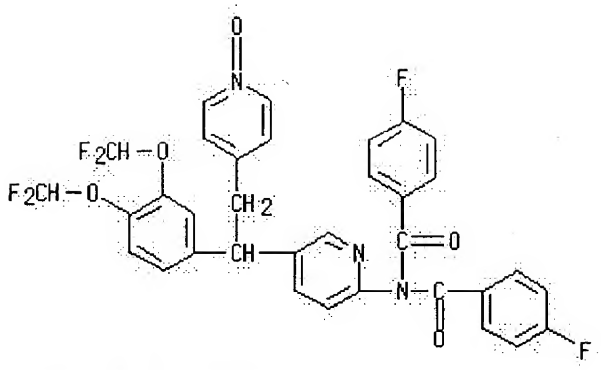

L12 ANSWER 62 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 2000:771978 HCAPLUS
DOCUMENT NUMBER: 134:71474
TITLE: Template-induced and molecular recognition directed hierarchical generation of supramolecular assemblies from molecular strands
AUTHOR(S): Berl, Volker; Krische, Michael J.; Huc, Ivan; Lehn, Jean-Marie; Schmutz, Marc
CORPORATE SOURCE: Laboratoire de Chimie Supramoleculaire, ESA 7006 of the CNRS, ISIS, Universite Louis Pasteur, Strasbourg, 67000, Fr.
SOURCE: Chemistry--A European Journal (2000), 6(11), 1938-1946
CODEN: CEUJED; ISSN: 0947-6539
PUBLISHER: Wiley-VCH Verlag GmbH
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 134:71474

AB A linear oligo-isophthalamide strand undergoes a conformational reorganization upon binding of 1-decylcyanuric acid to afford a helical disklike object possessing radially disposed alkyl residues. Solvophobic and stacking interactions drive a "second level" self-assembly of the templated structure, the stacking of the helical disks, to yield fibers as revealed by electron microscopy. These data provide insight into the interplay of the different structural and interactional features of the mol. components towards the formation of supramol. fibers through sequential hierarchical self-assembly events and suggest design strategies for the effector-controlled generation of related supramol. assemblies. The binding const. of 1-decylcyanuric acid for the linear oligo-isophthalamide strand was evaluated under various conditions by NMR and computational methods.

IT **315234-90-3**
RL: PRP (Properties)
(prepn. of supramol. assemblies by hydrogen-bonding and template-driven mol. assocn. of a isophthalamide-base mol. strand with a cyanuric acid deriv.)

RN 315234-90-3 HCAPLUS
CN 1,3-Benzenedicarboxamide, 5-(decyloxy)-N,N'-bis[6-[[3-(decyloxy)-5-[[[6-[(1-oxodecyl)]amino]-2-pyridinyl]amino]carbonyl]benzoyl]amino]-, compd. with 1-decyl-1,3,5-triazine-2,4,6(1H,3H,5H)-trione (1:2) (9CI) (CA INDEX NAME)

CM 1

CRN 315234-88-9
CMF C13 H23 N3 O3

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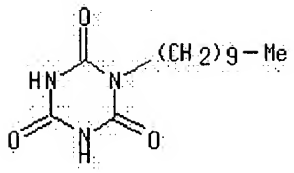
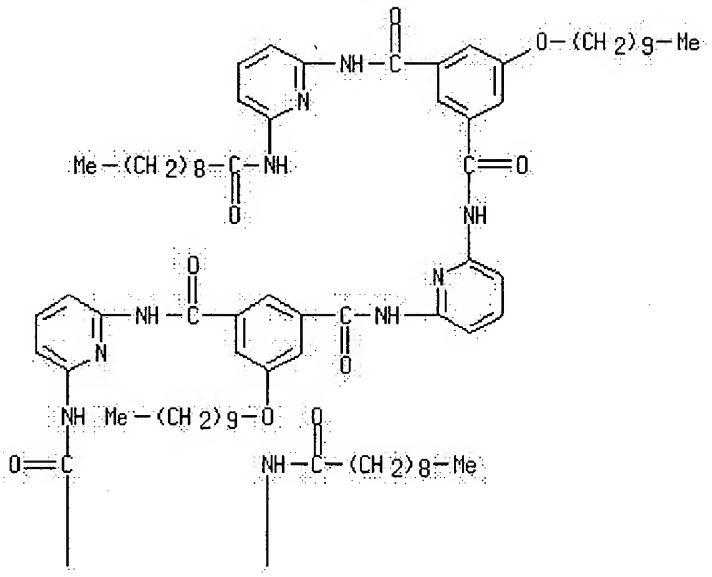


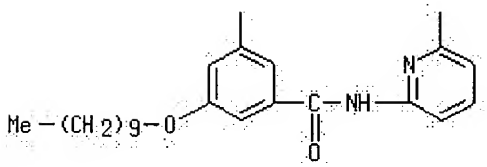
CM 2

CRN 315234-86-7
CMF C94 H130 N12 O11

PAGE 1-A



PAGE 2-A



REFERENCE COUNT: 44 THERE ARE 44 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 63 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Store Preferences

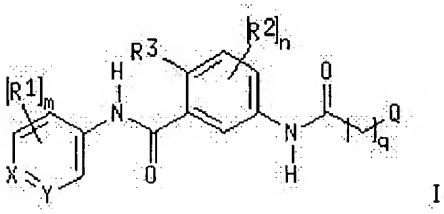
ACCESSION NUMBER: 2000:666695 HCAPLUS
DOCUMENT NUMBER: 133:252169
TITLE: Preparation of benzamides for treating diseases mediated by cytokines
INVENTOR(S): Brown, Dearg Sutherland
PATENT ASSIGNEE(S): Astrazeneca AB, Swed.
SOURCE: PCT Int. Appl., 96 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent

h eb c g cg b cg eb

LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000055120	A1	20000921	WO 2000-GB914	20000313
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
NZ 513726	A	20010928	NZ 2000-513726	20000313
EP 1163212	A1	20011219	EP 2000-909500	20000313
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
BR 2000009041	A	20011226	BR 2000-9041	20000313
TR 200102568	T2	20020521	TR 2001-200102568	20000313
JP 2002539187	T2	20021119	JP 2000-605551	20000313
AU 761291	B2	20030529	AU 2000-31780	20000313
ZA 2001006857	A	20021120	ZA 2001-6857	20010820
NO 2001004488	A	20011114	NO 2001-4488	20010914
US 6548514	B1	20030415	US 2001-936698	20010917
US 2003186966	A1	20031002	US 2003-353127	20030129
PRIORITY APPLN. INFO.:			GB 1999-6277 A	19990317
			GB 2000-2472 A	20000203
			WO 2000-GB914 W	20000313
			US 2001-936698 A3	20010917

OTHER SOURCE(S): MARPAT 133:252169
GI



I

AB The title compds. [I; X = CH, N; Y = CH, N; m = 0-3; R1 = OH, halo, CF3, etc.; n = 0-3; R2 = OH, halo, CF3, etc.; R3 = H, halo, alkyl, alkoxy; q = 0-4; Q = aryl, aryloxy, arylalkoxy, etc.], useful in the treatment of diseases or medical conditions mediated by cytokines, were prepd. and formulated. E.g., a multi-step synthesis of benzamide I [X, Y = CH; R1 = 4-Pr; m = 1; R2 = H; R3 = Me; q = 0; Q = 4-NCC6H4] was given. In general, compds. I give over 30% inhibition of p38α and/or p38β at up to 10 μM.

IT **295349-53-0P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of benzamides for treating diseases mediated by cytokines)

RN 295349-53-0 HCAPLUS

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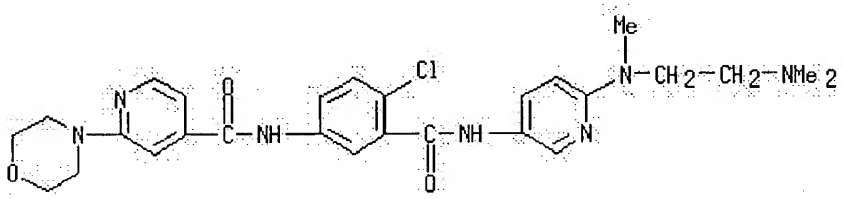
CN 4-Pyridinecarboxamide, N-[4-chloro-3-[[[6-[[2-(dimethylamino)ethyl]methylamino]-3-pyridinyl]amino]carbonyl]phenyl]-2-(4-morpholinyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 64 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

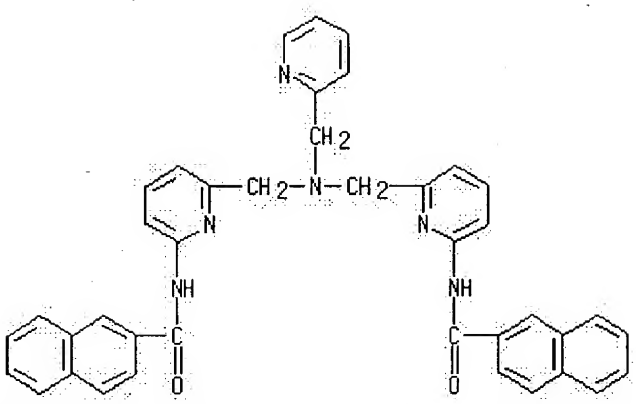
Full Text | Other References

ACCESSION NUMBER: 2000:651049 HCAPLUS
DOCUMENT NUMBER: 133:343788
TITLE: A ruthenium(II)-pyridylamine complex showing a fluxional intramolecular π-π interaction
AUTHOR(S): Kojima, Takahiko; Hayashi, Ken-Ichi; Matsuda, Yoshihisa
CORPORATE SOURCE: Department of Chemistry and Physics of Condensed Matter, Graduate School of Sciences, Kyushu University, Fukuoka, 812-8581, Japan
SOURCE: Chemistry Letters (2000), (9), 1008-1009
CODEN: CMLTAG; ISSN: 0366-7022
PUBLISHER: Chemical Society of Japan
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A novel ruthenium(II) complex having 2-naphthoylamide groups attached to TPA (tris(2-pyridylmethyl)amine), [RuCl(L)]PF6 (L = bis(6-(2-naphthoylamido)-2-pyridylmethyl)2-pyridylmethylamine) was synthesized and characterized by 1H NMR and x-ray crystallog. ([RuCl(L)]PF6·H2O·1/2EtOH: triclinic, space group P.hivin.1, R = 0.040). The 2-naphthoylamide arms exhibited fluxional behavior of intramol. π-π interaction.

IT **303187-36-2**
RL: RCT (Reactant); RACT (Reactant or reagent)
(for prepn. of ruthenium(II) bis(naphthoylamidopyridylmethyl)pyridylmethylamine chloro complex)

RN 303187-36-2 HCAPLUS
CN 2-Naphthalenecarboxamide, N,N'-[[(2-pyridinylmethyl)imino]bis(methylene-6,2-pyridinediyl)]bis- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 65 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Other References

ACCESSION NUMBER: 2000:609187 HCAPLUS
DOCUMENT NUMBER: 133:305278
TITLE: Classification of Some Active Compounds and Their Inactive Analogues Using Two Three-Dimensional Molecular Descriptors Derived from Computation of Three-Dimensional Convex Hulls for Structures Theoretically Generated for Them
AUTHOR(S): Lin, Thy-Hou; Yu, Yih-Shiang; Chen, Hong-Jih
CORPORATE SOURCE: Department of Life Science, National Tsing Hua University, Hsinchu, Taiwan
SOURCE: Journal of Chemical Information and Computer Sciences (2000), 40(5), 1210-1221
CODEN: JCISD8; ISSN: 0095-2338
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Two three-dimensional (3D) mol. descriptors are used to classify 73 protease inhibitors against the human immunodeficiency virus type 1 (HIV-1). X-ray structures of these HIV-1 protease bound inhibitors are used as templates to generate the most probable bioactive conformations of the inhibitors. A convex hull computation algorithm is applied to each structure generated. The frequency of atoms lying on the vertexes of each hull is counted. Vertexes of the same at. charge state are then gathered together as a set of commonly exposed groups for all the structures generated. The first 3D descriptor is computed as the max. mol. path length among any three distinct commonly exposed groups, while the second 3D one is computed as the max. mol. path length among any three atoms of nonconvex hull vertexes. We find that the 73 HIV-1 protease inhibitors can be classified by the first 3D descriptor into two groups, which agrees with the result of visual classification using the activity data as a criterion for these compds. The classification scheme is then used to classify a database of 427 active trypsin inhibitors and their inactive analogs. The structures of these compds. are generated theor. from steps of energy minimization and mol. dynamics. Classification for all these compds. is performed using the SYBYL hierarchical clustering method on the first 3D descriptor and then the second 3D one computed. It is found that some inactive analogs are completely sepd. from the active inhibitors at the first stage of classification using the first 3D descriptor. Most of the highly active inhibitors are classified into a cluster at the second stage of classification using the second 3D descriptor. Finally, most of

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these highly active inhibitors are sepd. from all the accompanying inactive analogs in the cluster through a structural alignment process using a set of commonly exposed groups detd. for them.

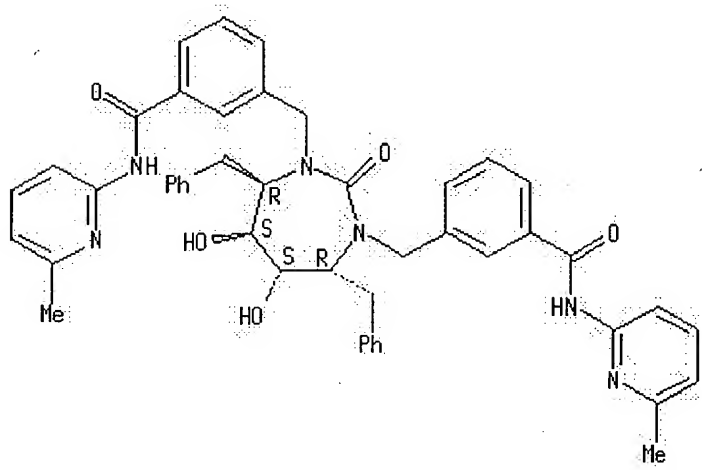
IT **183854-97-9**

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(three-dimensional mol. descriptors in classifying HIV-1 protease inhibitors)

RN 183854-97-9 HCAPLUS

CN Benzamide, 3,3'-[[(4R,5S,6S,7R)-tetrahydro-5,6-dihydroxy-2-oxo-4,7-bis(phenylmethyl)-1H-1,3-diazepine-1,3(2H)-diyl]bis(methylene)]bis[N-(6-methyl-2-pyridinyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 66 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 2000:553560 HCAPLUS
DOCUMENT NUMBER: 133:164005
TITLE: Preparation of substituted N-heterocyclyl benzamides and analogs as G-protein coupled heptahelical receptor binding compounds
INVENTOR(S): Shiosaki, Kazumi; Fleming, Paul
PATENT ASSIGNEE(S): Millennium Pharmaceuticals, Inc., USA
SOURCE: PCT Int. Appl., 80 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000046203	A2	20000810	WO 2000-US3042	20000203
WO 2000046203	A3	20010301		

W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI,

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SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ,
BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE,
DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF,
CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

EP 1150955 A2 20011107 EP 2000-907184 20000203
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
IE, SI, LT, LV, FI, RO

PRIORITY APPLN. INFO.: US 1999-118893P P 19990204
WO 2000-US3042 W 20000203

OTHER SOURCE(S): MARPAT 133:164005
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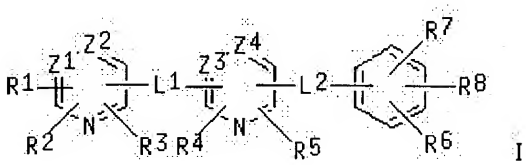

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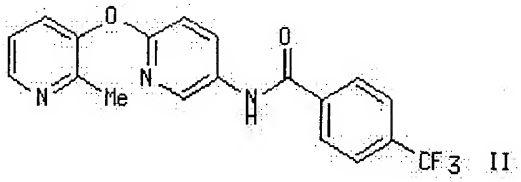
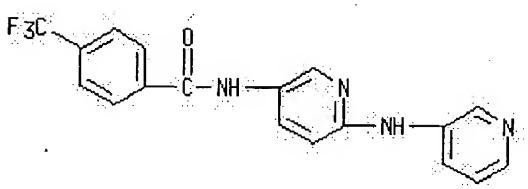


II

AB The title compds. (I) [wherein Z1-Z4 = independently N or C; R1-R8 = independently H, alkyl(amino), alkenyl, alkynyl, alkoxy, thioalkyl, hydroxyalkyl, halo(alkyl), NH2, or carboxyl; L1 = O, S, NH, NR7, (CHR7)n, C(O), CR7OH, or O(CHR7)n; n = 1-3; L2 = a bond, CH2C(O), NHC(O), OC(O), C(O), CH2NHC(O), NHC(O)CH2, CHOH, (CH2)n, O, NH, O(CH2)m, NH(CH2)m, CH2CHOH, and NR8C(O); m = 0-3] were prepd. for the treatment of neurol., immunol., inflammatory, cancer, and other β-chemokine mediated disorders. For example, coupling of 2-methyl-3-hydroxypyridine with 2-chloro-5-nitropyridine in the presence of NaH (87%), followed by redn. of the nitro group using Fe/AcOH (51%) and acylation of the amine with 4-trifluoromethylbenzoyl chloride, gave II. In a time resolved fluorescence (TRF) assay, II showed very high binding affinity for the CCR10 receptor with IC50 of < 5 μM.

IT 287943-06-0P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(GPCR binding compd.; prepn. of substituted N-heterocyclyl benzamide β-chemokine antagonists and analogs by coupling hydroxyheterocycles with 2-chloro-5-nitroheterocycles, redn. to the amines, and acylation with benzoyl chlorides)

RN 287943-06-0 HCAPLUS
CN Benzamide, N-[6-(3-pyridinylamino)-3-pyridinyl]-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)



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L12 ANSWER 67 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | More References

ACCESSION NUMBER: 2000:457059 HCAPLUS
DOCUMENT NUMBER: 133:89437
TITLE: Preparation of heteroaryl-substituted aromatic amides as factor Xa inhibitors
INVENTOR(S): Beight, Douglas Wade; Craft, Trelia Joyce; Denny, Carl Penman; Franciskovich, Jeffry Bernard; Goodson, Theodore, Jr.; Hall, Steven Edward; Herron, David Kent; Joseph, Sajan Pariyadan; Klimkowski, Valentine Joseph; Masters, John Joseph; Mendel, David; Milot, Guy; Pineiro-Nunez, Marta Maria; Sawyer, Jason Scott; Shuman, Robert Theodore; Smith, Gerald Floyd; Tebbe, Anne Louise; Tinsley, Jennifer Marie; Weir, Leonard Crayton; Wikel, James Howard; Wiley, Michael Robert; Yee, Ying Kwong
PATENT ASSIGNEE(S): Eli Lilly and Co., USA; Kyle, Jeffrey, Alan; et al.
SOURCE: PCT Int. Appl., 403 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000039118	A1	20000706	WO 1999-US29946	19991215
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
CA 2361149	AA	20000706	CA 1999-2361149	19991215
EP 1140903	A1	20011010	EP 1999-964279	19991215
EP 1140903	B1	20040804		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
JP 2002533454	T2	20021008	JP 2000-591029	19991215
US 6635657	B1	20031021	US 2001-857751	20010608
US 2004029874	A1	20040212	US 2003-629760	20030729
US 6759414	B2	20040706		

PRIORITY APPLN. INFO.:	US 1998-113556P	P	19981223
	WO 1999-US29946	W	19991215
	US 2001-857751	A3	20010608

OTHER SOURCE(S): MARPAT 133:89437
GI

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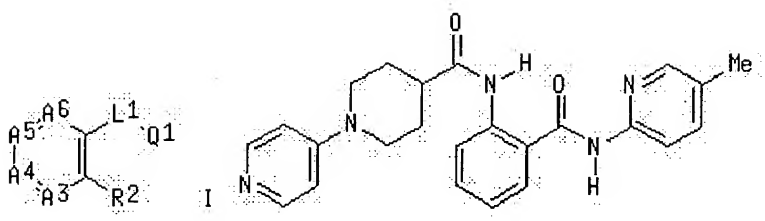


AB The title compds. [I; A3-A6, together with the two carbons to which they are attached, complete a substituted benzene in which A3 = CR3, A4 = CR4, A5 = CR5, and A6 = CR6 (wherein R3 = H, Me, MeO, etc.; one of R4 and R5 = H, alkyl, halo, etc.; the other of R4 and R5 = H; R6 = H, Me, F, etc.); L1 = CONH; Q1 = 2-pyridinyl (un)substituted at the 5-position, 3-pyridinyl (un)substituted at the 6-position, 2-pyrimidinyl (un)substituted at the 5-position, etc.; R2 = L2Q2 (L2 = NHCO, NHCH2, OCH2, etc.; Q2 = (un)substituted piperidinyl, piperazinyl, Ph, etc.)] and their pharmaceutically acceptable salts, useful as inhibitors of factor Xa (no data), were prepd. and formulated. E.g., a multi-step synthesis of II.HCl was given. In general, compds. I are effective at 0.01-1000 mg/kg/day.

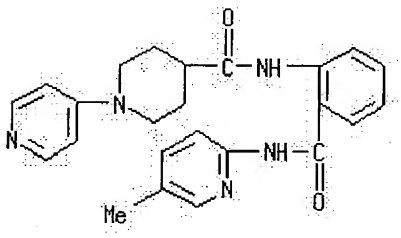
IT **280768-65-2P**

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of heteroaryl-substituted arom. amides as factor Xa inhibitors)

RN 280768-65-2 HCAPLUS

CN 4-Piperidinecarboxamide, N-[2-[[(5-methyl-2-pyridinyl)amino]carbonyl]phenyl]-1-(4-pyridinyl)-, dihydrochloride (9CI) (CA INDEX NAME)



2 HCl

REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 68 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Cited References

ACCESSION NUMBER: 2000:457058 HCAPLUS

DOCUMENT NUMBER: 133:73942

TITLE: Preparation of heteroroaromatic amides as factor Xa inhibitors

INVENTOR(S): Beight, Douglas Wade; Craft, Trelia Joyce; Franciskovich, Jeffry Bernard; Goodson, Theodore, Jr.; Hall, Steven Edward; Herron, David Kent; Joseph, Sajan Pariyadan; Klimkowski, Valentine Joseph; Masters, John Joseph; Mendel, David; Milot, Guy; Pineiro-Nunez, Marta Maria; Sawyer, Jason Scott; Shuman, Robert Theodore; Smith, Gerald Floyd; Tebbe, Anne Louise; Tinsley, Jennifer Marie; Weir, Leonard Crayton; Wikel, James Howard; Wiley, Michael Robert; Yee, Ying Kwong

h eb c g cg b cg eb

PATENT ASSIGNEE(S): Eli Lilly and Company, USA; Kyle, Jeffrey Alan
SOURCE: PCT Int. Appl., 93 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 2000039117	A1	20000706	WO 1999-US29887		19991215
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM					
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG					
CA 2358095	AA	20000706	CA 1999-2358095		19991215
EP 1140905	A1	20011010	EP 1999-967352		19991215
EP 1140905	B1	20030514			
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AT 240316	E	20030515	AT 1999-967352		19991215
ES 2196917	T3	20031216	ES 1999-967352		19991215
US 6689780	B1	20040210	US 2001-857749		20010608
PRIORITY APPLN. INFO.:			US 1998-113452P	P	19981223
			EP 1999-967352	A	19991215
			WO 1999-US29887	W	19991215

OTHER SOURCE(S): MARPAT 133:73942
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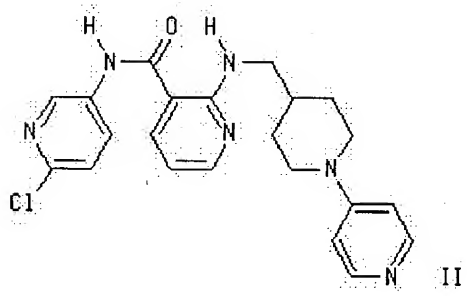


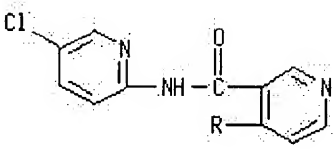
II

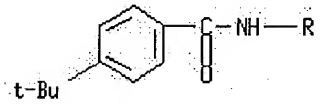
AB R2Z2ZCONHZ1R1 [I; R1 = Cl, F, Me; R2 = N-(un)substituted azacycloalkyl, 4-(un)substituted -1-piperazinyl, 4-aminocyclohexyl, 4-amino-1-piperidinyl, etc.; Z = (un)substituted-2,3- or -3,2-pyridinediyl, -5,4- or -4,5-pyrimidinediyl, -2,3-pyrazinediyl, etc.; Z1 = 2,5-pyridinediyl (R1 may addnl. = MeO or MeS), 2,5-pyrimidinediyl, 3,6-pyridazinediyl, 2,6-benzothiazolediyl; Z2 = NHCOX, NHCO2X, NHCONHX, NHCH2; X = bond or CH2] were prepd. as factor Xa inhibitors (no data). Thus, 2-chloronicotinic acid was aminated by 1-(4-pyridinyl)piperidine-4-methylamine (prepn. given) and the product amidated by 2-amino-5-chloropyridine to give title compd. II.

IT **280115-68-6P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

h eb c g cg b cg eb

(prepn. of heteroroarom. amides as factor Xa inhibitors)
RN 280115-68-6 HCAPLUS
CN 3-Pyridinecarboxamide, N-(5-chloro-2-pyridinyl)-4-[[4-(1,1-dimethylethyl)benzoyl]amino]- (9CI) (CA INDEX NAME)





REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 69 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 2000:457052 HCAPLUS
DOCUMENT NUMBER: 133:89436
TITLE: Antithrombotic aryl amides and their preparation
INVENTOR(S): Beight, Douglas Wade; Craft, Trelia Joyce; Franciskovich, Jeffry Bernard; Goodson, Theodore, Jr.; Hall, Steven Edward; Herron, David Kent; Joseph, Sajan; Klimkowski, Valentine Joseph; Masters, John Joseph; Mendel, David; Milot, Guy; Pineiro-Nunez, Marta Maria; Sawyer, Jason Scott; Shuman, Robert Theodore; Smith, Gerald Floyd; Tebbe, Anne Louise; Tinsley, Jennifer Marie; Weir, Leonard Crayton; Wikel, James Howard; Wiley, Michael Robert; Yee, Ying Kwong
PATENT ASSIGNEE(S): Eli Lilly and Company, USA; Kyle, Jeffrey Alan
SOURCE: PCT Int. Appl., 80 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000039111	A1	20000706	WO 1999-US29832	19991215
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
CA 2358091	AA	20000706	CA 1999-2358091	19991215
EP 1140881	A1	20011010	EP 1999-964269	19991215
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
JP 2004522689	T2	20040729	JP 2000-591022	19991215

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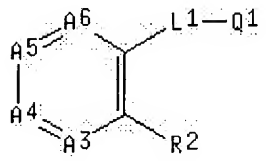
US 6610704	B1	20030826	US 2001-857747		20010608
US 2003191153	A1	20031009	US 2003-374124		20030225
US 6716855	B2	20040406			
US 2003199505	A1	20031023	US 2003-378108		20030226
US 6716839	B2	20040406			
US 2003199504	A1	20031023	US 2003-377906		20030228
US 6710057	B2	20040323			
US 2003212069	A1	20031113	US 2003-382614		20030305
US 6780878	B2	20040824			
PRIORITY APPLN. INFO.:			US 1998-113778P	P	19981223
			WO 1999-US29832	W	19991215
			US 2001-857747	A3	20010608

OTHER SOURCE(S): CASREACT 133:89436; MARPAT 133:89436

GI



I

AB Title compds. I [A3-A6, together with the 2 C atoms to which they are attached, form a substituted benzene, A3 = CR3, A4 = CR4, A5 = CR5, A6 = CR6, R3 = H, R4 or R5 = H, Me, F, Cl, carboxy, alkoxycarbonyl, amino, sulfonylamido, and the other of R4 or R5 = H, R6 = H; A3-A6, together with the 2 C atoms to which they are attached, form a substituted heteroarom. ring in which either one of A3-A6 = N and the others = CR3-CR6, or 2 non-adjacent A3-A6 are each N, and each of the others is CR3-CR6, resp., where R3-R6 = H, Me, or 1 of R3-R6 attached to a C not bonded to an N is Cl and the others are H, preferably, none of A3-A6 = N and each of R3-R6 = H, or each of R3, R4 and R6 = H and R5 = Cl, or A3 = N and each of A4-A6 = CH; L1 = NHCO, CONH, CH2NH; Q1 = (un)substituted Ph, 2-furanyl, 2-thienyl, 4-thiazolyl, 2-pyridyl, 2-naphthyl, 1,2-dihydrobenzofuran-5-yl or -6-yl, 1,2-benzisoxazol-6-yl, 6-indolyl, 6-indolinyl, 6-indazolyl, 5-benzimidazolyl, 5-benzotriazolyl; R2 = NHCH2Q2, Q2 = substituted Ph or (un)substituted 4-piperidinyl, preferably, R2 = 4-(4-morpholinyl)benzylamino, [1-(4-pyridinyl)piperidin-4-ylmethyl]amino, (1-isopropylpiperidin-4-ylmethyl)amino] or their pharmaceutically acceptable salts and pharmaceutical compns., useful as inhibitors of blood-coagulation factor Xa (no data), are claimed, along with a process for their prepn. and synthetic intermediates. In an example, I [A3 = N, A4-A6 = CH; L1 = NHCO; Q1 = 4-MeOC6H4; R2 = [1-(4-pyridinyl)piperidin-4-ylmethyl]amino] is prepd. in 3 steps starting from 2-chloro-3-nitropyridine and 1-(4-pyridyl)piperidine-4-methylamine (prepn. given).

IT **280556-53-8P**

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of aryl amides as antithrombotics)

RN 280556-53-8 HCAPLUS

CN Benzamide, 4-methoxy-N-[2-[[[1-(4-pyridinyl)-4-piperidinyl]methyl]amino]-3-pyridinyl]- (9CI) (CA INDEX NAME)

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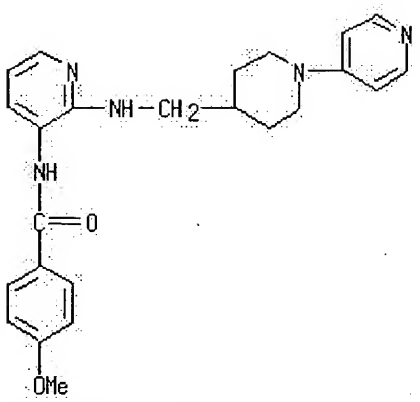

REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 70 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Hitlist References

ACCESSION NUMBER: 2000:335387 HCAPLUS
DOCUMENT NUMBER: 132:334364
TITLE: Preparation of anthranilic acid amides as vascular endothelial growth factor receptor inhibitors.
INVENTOR(S): Huth, Andreas; Seidelmann, Dieter; Thierauch, Karl-Heinz; Bold, Guido; Manley, Paul William; Furet, Pascal; Wood, Jeanette Marjorie; Mestan, Jurgen; Bruggen, Jose; Ferrari, Stefano; Kruger, Martin; Ottow, Eckhard; Menrad, Andreas; Schirner, Michael
PATENT ASSIGNEE(S): Schering Aktiengesellschaft, Germany; Novartis Aktiengesellschaft
SOURCE: PCT Int. Appl., 96 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000027819	A2	20000518	WO 1999-EP8478	19991109
WO 2000027819	A3	20000817		
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
DE 19910396	A1	20000907	DE 1999-19910396	19990303
DE 19910396	C2	20011213		
BR 9915553	A	20010814	BR 1999-15553	19991109
EP 1129074	A2	20010905	EP 1999-953967	19991109
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
TR 200101307	T2	20020521	TR 2001-200101307	19991109
JP 2002529452	T2	20020910	JP 2000-580999	19991109
EE 200100258	A	20021216	EE 2001-258	19991109

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NZ 511413	A	20040130	NZ 1999-511413		19991109
AU 771180	B2	20040318	AU 2000-10454		19991109
NO 2001002245	A	20010710	NO 2001-2245		20010507
BG 105588	A	20020430	BG 2001-105588		20010611
PRIORITY APPLN. INFO.:			GB 1998-24579	A	19981110
			DE 1999-19910396	A	19990303
			WO 1999-EP8478	W	19991109

OTHER SOURCE(S): MARPAT 132:334364

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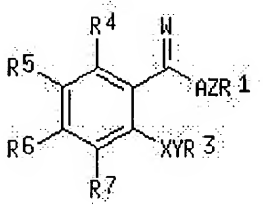


I

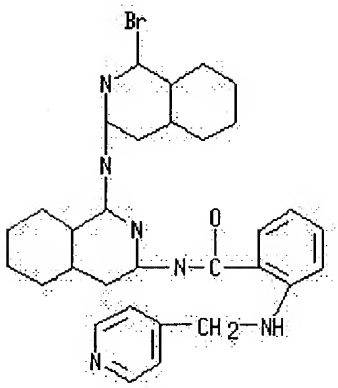
AB Title compds. [I; A = NR2; W = O, S, H2, NR8; Z = NR10, N, NR10(CH2)q, alkyl, etc.; q = 1-6; AZR1 = tetrahydroisoquinolinyl, indazolyl, 5-chloroindolyl, etc.; R1 = (substituted) aryl, heteroaryl; R2 = H, alkyl; R3 = (substituted) mono- or bicyclic aryl, heteroaryl; R4-R7 = H, halo, (substituted) alkoxy, alkyl, carboxyalkyl; R5R6 = dioxetanyl; R8, R10 = H, alkyl]. Thus, Me N-(4-pyridylmethyl)anthranilate (prepn. given) was stirred with Ph(CH2)3NH2 and Me3Al were stirred in PhMe to give N-(3-phenylprop-1-yl)-N2-(4-pyridylmethyl)anthranilamide. The latter inhibited VEGFR I with IC50 = 0.05 μM.

IT **267891-25-8P**

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of anthranilic acid amides as VEGF receptor inhibitors)

RN 267891-25-8 HCAPLUS

CN Benzamide, N-[1-[(1-bromo-3-isoquinolinyl)amino]-3-isoquinolinyl]-2-[(4-pyridinylmethyl)amino]- (9CI) (CA INDEX NAME)



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L12 ANSWER 71 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Cited References

ACCESSION NUMBER: 2000:196152 HCAPLUS
Correction of: 1999:784096

DOCUMENT NUMBER: 132:194297
Correction of: 132:12266

h eb c g cg b cg eb

TITLE: Preparation of N-acylarylalanines as α4 integrin antagonists
INVENTOR(S): Head, John Clifford; Warrellow, Graham John; Porter, John Robert; Archibald, Sarah Catherine
PATENT ASSIGNEE(S): Celltech Therapeutics Limited, UK
SOURCE: PCT Int. Appl., 47 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9962901	A1	19991209	WO 1999-GB1741	19990603
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
US 6110945	A	20000829	US 1999-323966	19990602
CA 2331791	AA	19991209	CA 1999-2331791	19990603
AU 9941566	A1	19991220	AU 1999-41566	19990603
AU 765979	B2	20031009		
EP 1084119	A1	20010321	EP 1999-925183	19990603
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JP 2002517391	T2	20020618	JP 2000-552112	19990603
US 6369229	B1	20020409	US 2000-538918	20000330

PRIORITY APPLN. INFO.:

GB 1998-11969	A	19980603
US 1999-323966	A3	19990602
WO 1999-GB1741	W	19990603

OTHER SOURCE(S): MARPAT 132:194297
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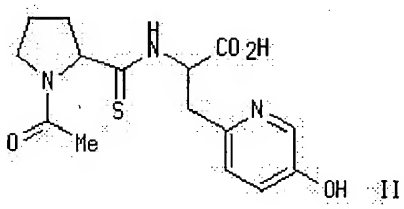


II

AB R1Z1ZZ2Z3CRR4R5 [I; R = CO2 or deriv. thereof (sic); R1 = H, (hetero)cycloaliph. group, (hetero)aryl; R4 = H or Me; R5 = NHCOR6, NHCSR6, etc.; R6 = (hetero)(cyclo)aliph. group, (hetero)aryl, etc.; Z = bond or linker atom or group (sic); Z1 = bond, divalent (hetero)aliph. group; Z2 = pyridinediyl, pyrimidinediyl, pyrazinediyl, etc.; Z3 = bond or alkylene] were prepd. Thus, Ph2CHNHCH2CO2Et was alkylated by 2-bromomethyl-5-phenylsulfonyloxypyridine and the N-deprotected product acylated by N-acetyl-D-thioproline to give, after sapon., a diastereomeric mixt. of title compd. II. Data for biol. activity of I were given.

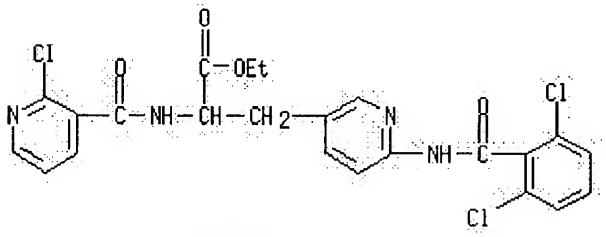
IT **251458-86-3P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);

h eb c g cg b cg eb

BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of N-acylarylalanines as α4 integrin antagonists)

RN 251458-86-3 HCAPLUS

CN 3-Pyridinepropanoic acid, α-[[(2-chloro-3-pyridinyl)carbonyl]amino]-6-[(2,6-dichlorobenzoyl)amino]-, ethyl ester (9CI) (CA INDEX NAME)



L12 ANSWER 72 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | More References

ACCESSION NUMBER:	2000:145222 HCAPLUS
DOCUMENT NUMBER:	132:278892
TITLE:	Troger's Base Molecular Scaffolds in Dicarboxylic Acid Recognition
AUTHOR(S):	Goswami, Shyamaprosad; Ghosh, Kumaresh; Dasgupta, Swagata
CORPORATE SOURCE:	Department of Chemistry, Bengal Engineering College (Deemed University) Botanic Garden, Howrah, 711 103, India
SOURCE:	Journal of Organic Chemistry (2000), 65(7), 1907-1914 CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER:	American Chemical Society
DOCUMENT TYPE:	Journal
LANGUAGE:	English

GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Artificial receptors (I,II,III,IV,and V) have been designed and synthesized from simple precursors. The chain length selectivity studies of dicarboxylic acids within the cavities of new fluorescent Troger's base mol. frameworks (I, II,and III) have been carried out with a crit. examn. of their role of rigidity as well as flexibility in selective binding in comparison to receptor V. The chiral resoln. of the racemic Troger's base receptors (I and II) by chiral recognition with (+)- camphoric acid using hydrogen-bonding interactions has been studied.

IT **263909-11-1P**

RL: PEP (Physical, engineering or chemical process); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)
(Troger's base mol. scaffolds in dicarboxylic acid recognition)

RN 263909-11-1 HCAPLUS

CN Benzamide, 3,3'-(1,2-ethanediyl)bis[N-(6-methyl-2-pyridinyl)- (9CI) (CA INDEX NAME)

h eb c g cg b cg eb

LANGUAGE: English

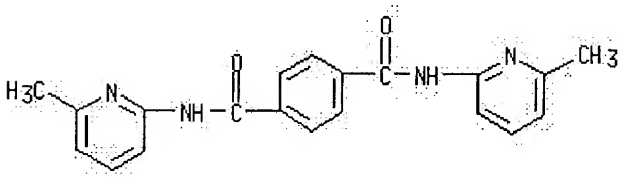
AB Supramol. effects on the intramol. Diels-Alder (IMDA) reaction of substituted furfurylfumaramides are studied using a series of synthetic receptors with differentially positioned hydrogen bonding groups. Using temp. jump techniques, an increase of up to 30-fold in the rate of the IMDA reaction was detd. for a receptor that is complementary to the transition state structure compared to one that binds most strongly to the starting material.

IT **129708-38-9**

RL: PRP (Properties)
(effect of, on intramol. Diels-Alder reaction of furfurylfumaramide)

RN 129708-38-9 HCAPLUS

CN 1,4-Benzenedicarboxamide, N,N'-bis(6-methyl-2-pyridinyl)- (9CI) (CA INDEX NAME)



L12 ANSWER 143 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 1990:631636 HCAPLUS

DOCUMENT NUMBER: 113:231636

TITLE: Hydrogen-bonding self-assembly of multichromophore structures

AUTHOR(S): Tecilla, Paolo; Dixon, Robert P.; Slobodkin, Gregory; Alavi, David S.; Waldeck, David H.; Hamilton, Andrew D.

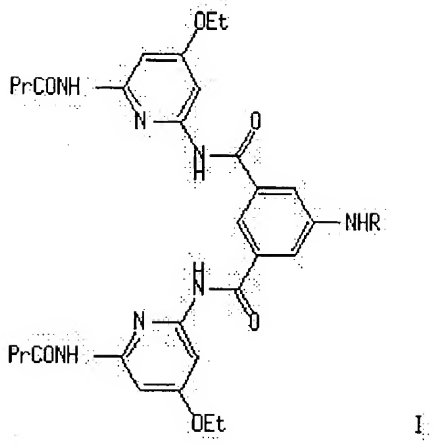
CORPORATE SOURCE: Dep. Chem., Univ. Pittsburgh, Pittsburgh, PA, 15260, USA

SOURCE: Journal of the American Chemical Society (1990), 112(25), 9408-10
CODEN: JACSAT; ISSN: 0002-7863

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



I

AB Complementary hydrogen bonding groups have been covalently linked to

h eb c g cg b cg eb

different redox or photoactive chromophores, e.g., I (R = ferrocenylcarbonyl). Static dynamic fluorescence spectroscopic studies show that matched subunits will self-assemble in soln. (at 10-5-10-6 M) to form multichromophore aggregates with energy transfer quenching between the chromophores.

IT **130350-29-7P**

RL: PRP (Properties); PREP (Preparation)
(formation and fluorescence of)

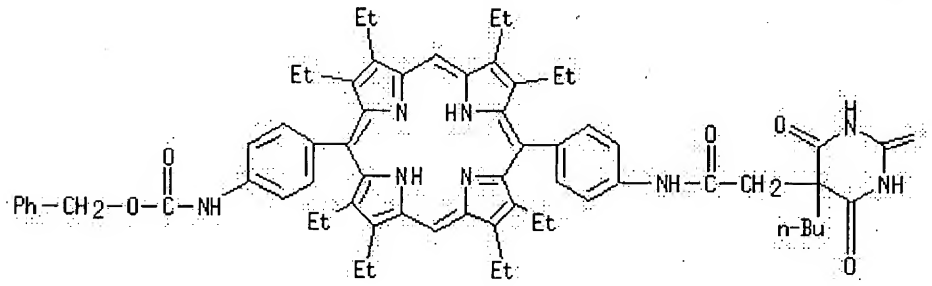
RN 130350-29-7 HCAPLUS

CN Carbamic acid, [4-[15-[4-[[(5-butylhexahydro-2,4,6-trioxo-5-pyrimidinyl)acetyl]amino]phenyl]-2,3,7,8,12,13,17,18-octaethyl-21H,23H-porphin-5-yl]phenyl]-, phenylmethyl ester, compd. with 5-[[[5-(dimethylamino)-1-naphthalenyl]sulfonyl]amino]-N,N'-bis[4-ethoxy-6-[(1-oxobutyl)amino]-2-pyridinyl]-1,3-benzenedicarboxamide (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 130326-58-8
CMF C66 H74 N8 O6

PAGE 1-A



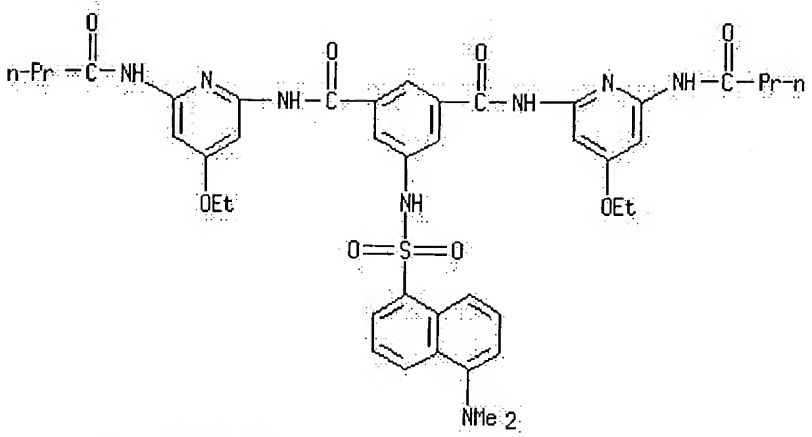
PAGE 1-B

=O

CM 2

CRN 130326-57-7
CMF C42 H48 N8 O8 S

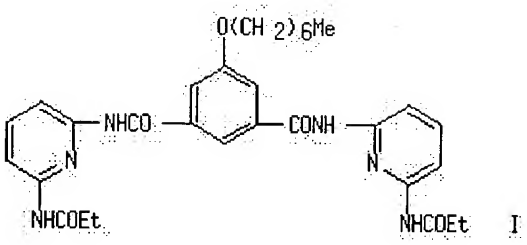
h eb c g cg b cg eb



L12 ANSWER 144 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 1990:627003 HCAPLUS
DOCUMENT NUMBER: 113:227003
TITLE: Transition-state stabilization and molecular recognition: acceleration of phosphoryl-transfer reactions by an artificial receptor
AUTHOR(S): Tecilla, Paolo; Chang, Suk Kyu; Hamilton, Andrew D.
CORPORATE SOURCE: Dep. Chem., Univ. Pittsburgh, Pittsburgh, PA, 15260, USA
SOURCE: Journal of the American Chemical Society (1990), 112(26), 9586-90
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



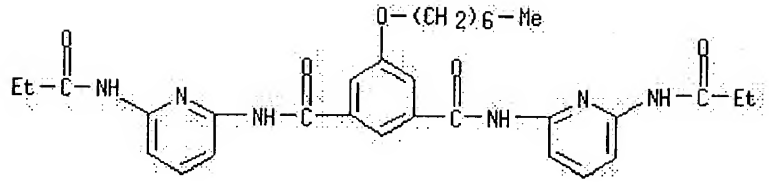
I

AB An artificial receptor (I) that is complementary to the proposed trigonal-bipyramidal intermediate for phosphoryl-transfer reactions has been designed. Kinetic measurements with 31P NMR methods show that the receptor causes up to a 10-fold acceleration in the aminolysis of phosphorodiamidic chloride derivs., proceeding via an associative mechanism.

IT **129648-66-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and phosphoryl transfer reaction acceleration by, transition state stabilization and enzymic reaction mechanisms in relation to)

RN 129648-66-4 HCAPLUS
CN 1,3-Benzenedicarboxamide, 5-(heptyloxy)-N,N'-bis[6-[(1-oxopropyl)amino]-2-pyridinyl]- (9CI) (CA INDEX NAME)

h eb c g cg b cg eb



L12 ANSWER 145 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 1990:571401 HCAPLUS
DOCUMENT NUMBER: 113:171401
TITLE: Molecular recognition: a remarkably simple receptor for the selective complexation of dicarboxylic acids
AUTHOR(S): Garcia-Tellado, Fernando; Goswami, Shyamaprosad; Chang, Suk Kyu; Geib, Steven J.; Hamilton, Andrew D.
CORPORATE SOURCE: Dep. Chem., Univ. Pittsburgh, Pittsburgh, PA, 15260, USA
SOURCE: Journal of the American Chemical Society (1990), 112(20), 7393-4
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: English

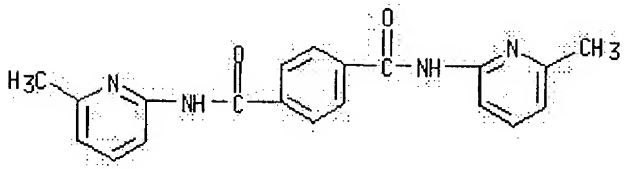
AB A new and remarkably simple receptor for dicarboxylic acids is prepd. from the reaction of 2-amino-6-methylpyridine and terephthaloyl dichloride. 1H NMR and x-ray crystallog. studies on the complex confirm the formation of four hydrogen bonds and the position of the alkyl chain beneath the benzene ring.

IT **129708-40-3**
RL: PRP (Properties)
(formation const. of)

RN 129708-40-3 HCAPLUS
CN Pentanedioic acid, compd. with N,N'-bis(6-methyl-2-pyridinyl)-1,4-benzenedicarboxamide (1:1) (9CI) (CA INDEX NAME)

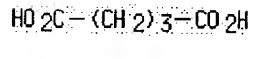
CM 1

CRN 129708-38-9
CMF C20 H18 N4 O2



CM 2

CRN 110-94-1
CMF C5 H8 O4



L12 ANSWER 146 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

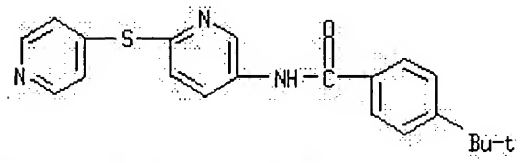
Full Text | Citing References

h eb c g cg b cg eb

ACCESSION NUMBER: 1990:76956 HCAPLUS
DOCUMENT NUMBER: 112:76956
TITLE: Preparation of tertiary-butylphenylcarbamoylpyridines as cardiovascular agents
INVENTOR(S): Von der Saal, Wolfgang; Mertens, Alfred; Zilch, Harald; Boehm, Erwin; Martin, Ulrich
PATENT ASSIGNEE(S): Boehringer Mannheim G.m.b.H., Fed. Rep. Ger.
SOURCE: Ger. Offen., 13 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 3804346	A1	19890824	DE 1988-3804346	19880212
PRIORITY APPLN. INFO.:			DE 1988-3804346	19880212

OTHER SOURCE(S): CASREACT 112:76956; MARPAT 112:76956
GI For diagram(s), see printed CA Issue.
AB The title compds. [I; R1 = H, alkyl, alkenyl, alkynyl, cycloalkyl, cycloalkenyl, halo, OH, alkoxy, alkenyloxy, alkynyloxy, cycloalkoxy, cycloalkenyloxy, alkylthio, imidazolyl, triazolyl, morpholinyl, thiomorphilinyl, (substituted) pyridinyloxy, pyridinylthio, quinolinyloxy, naphthyloxy, indolyloxy, oxindolyloxy, etc.; A-B = CONH, NHCO]; useful as cardiovascular agents (no data), were prepd. Thus, 4-Me3CC6H4COCl in CH2Cl2 was added to 5-amino-2-(1-cyanophenyloxy)pyridine and Et3N in CH2Cl2 with ice cooling. The mixt. was stirred 10 min at room temp. to give 23% 4-tert-butyl-N-[6(4-cyanophenyloxy)-3-pyridinyl)benzamide.
IT **125125-24-8P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of, as cardiovascular agent)
RN 125125-24-8 HCAPLUS
CN Benzamide, 4-(1,1-dimethylethyl)-N-[6-(4-pyridinylthio)-3-pyridinyl]- (9CI) (CA INDEX NAME)

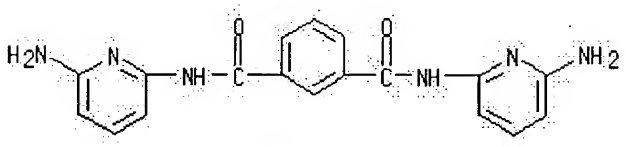


L12 ANSWER 147 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN
Full Text | Citing References

ACCESSION NUMBER: 1989:589885 HCAPLUS
DOCUMENT NUMBER: 111:189885
TITLE: Nucleotide recognition by macrocyclic receptors
AUTHOR(S): Hamilton, Andrew D.; Muehldorf, Alex; Chang, Suk Kyu; Pant, Nalin; Goswami, Shyamaprosad; Van Engen, Donna
CORPORATE SOURCE: Dep. Chem., Princeton Univ., Princeton, NJ, 08544, USA
SOURCE: Journal of Inclusion Phenomena and Molecular Recognition in Chemistry (1989), 7(1), 27-38
CODEN: JIMCEN; ISSN: 0167-7861
DOCUMENT TYPE: Journal
LANGUAGE: English

h eb c g cg b cg eb

OTHER SOURCE(S): CASREACT 111:189885
AB Complementary positioning of recognition sites (particularly H bonding, stacking and hydrophobic groups) into a macrocyclic receptor structure can lead to very strong and specific complexation of uncharged org. mols.
IT **112817-57-9**
RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation of, with acid chlorides)
RN 112817-57-9 HCAPLUS
CN 1,3-Benzenedicarboxamide, N,N'-bis(6-amino-2-pyridinyl)- (9CI) (CA INDEX NAME)



L12 ANSWER 148 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 1988:630812 HCAPLUS
DOCUMENT NUMBER: 109:230812
TITLE: Preparation of N,N'-bis(pyridyl- and pyrazinylalkyl)diimides as materials for polymers and dyes
INVENTOR(S): Niwa, Takakazu; Kurohara, Takayuki; Motoyama, Yukio
PATENT ASSIGNEE(S): Koei Chemical Industry Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 5 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 63091384	A2	19880422	JP 1986-238661	19861007
JP 07025751	B4	19950322		
PRIORITY APPLN. INFO.:			JP 1986-238661	19861007

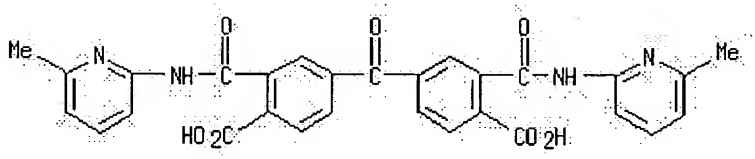
OTHER SOURCE(S): CASREACT 109:230812; MARPAT 109:230812
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Title compds. I (R1, R2 = H, C1-3 alkyl, PhCH2; X = CH, N; R = C6H2, C6H3C6H3, C6H3COC6H3, C6H3OC6H3; n = 0, 1) are prepd. either directly or via amide II by condensation of dicarboxylic acid anhydride III and amine IV. A mixt. of 2-amino-6-picoline 4.32, 3,3',4,4'-benzophenonetetracarboxylic dianhydride 6.44, and 3,5-lutidine 70 g was heated at 170° with removal of the produced H2O to give 9.5 g imide V.
IT **117702-90-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, as intermediate for diimide)
RN 117702-90-6 HCAPLUS
CN Benzoic acid, 4,4'-carbonylbis[2-[[(6-methyl-2-pyridinyl)amino]carbonyl]-

h eb c g cg b cg eb

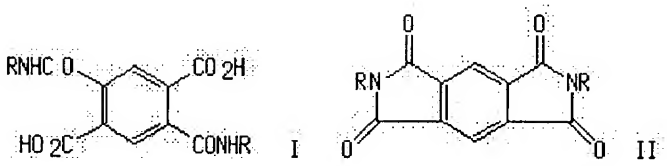
(9CI) (CA INDEX NAME)



L12 ANSWER 149 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Cited References

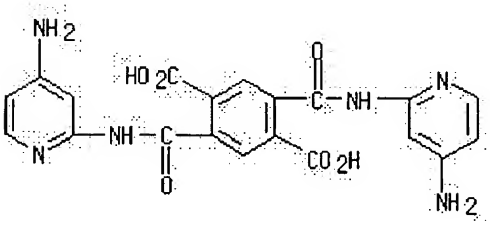
ACCESSION NUMBER: 1988:416608 HCAPLUS
DOCUMENT NUMBER: 109:16608
TITLE: The synthesis of pyromellitamic diacids and pyromellitdiimides and their effect on the human serum cholinesterase activity in vitro
AUTHOR(S): Al-Azzawi, Mohammad J.; Atto, Amir T.; Al-Ahdami, Balqiz W.; Ali, Imad T.
CORPORATE SOURCE: Biol. Res. Cent., Baghdad, Iraq
SOURCE: Journal of Biological Sciences Research (1988), 19(1), 85-93
CODEN: JBSREF; ISSN: 1012-344X
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



AB Eight pyromellitamic diacids I (R = substituted Ph or pyridyl or tetrazyl) were prepd. by reaction of amines with pyromellitic dianhydride and then 4 of them were cyclized by dehydration with the acetic anhydride-sodium acetate system to form the corresponding diimides II (R = substituted phenyl). I and II dose-dependently inhibited cholinesterase of human blood serum.

IT **114932-56-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and cholinesterase of blood serum of humans inhibition by and cyclization of)

RN 114932-56-8 HCAPLUS
CN 1,4-Benzenedicarboxylic acid, 2,5-bis[[(4-amino-2-pyridinyl)amino]carbonyl]- (9CI) (CA INDEX NAME)



h eb c g cg b cg eb

L12 ANSWER 150 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

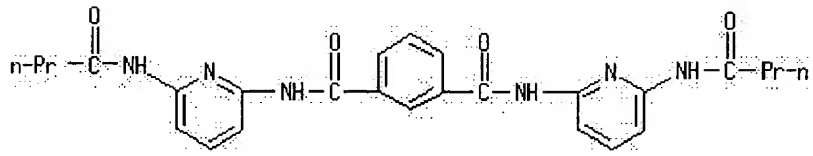
ACCESSION NUMBER: 1988:112419 HCAPLUS
DOCUMENT NUMBER: 108:112419
TITLE: Molecular recognition of biologically interesting substrates: synthesis of an artificial receptor for barbiturates employing six hydrogen bonds
AUTHOR(S): Chang, Suk Kyu; Hamilton, Andrew D.
CORPORATE SOURCE: Dep. Chem., Princeton Univ., Princeton, NJ, 08544, USA
SOURCE: Journal of the American Chemical Society (1988), 110(4), 1318-19
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 108:112419
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The synthesis and binding properties of the macrocycle I, a novel receptor for barbiturates, is reported. Thus, 3-ClCOC6H4COCl was treated with 2,6-diaminopyridine and Et3N in THF to give 79% the bis(aminopyridyl)isophthalamide II (R = H), which cyclocondensed with 4-ClCO(CH2)3OC6H4CMe2C6H4O(CH2)3COCl-4 in THF-Et3N at high diln. to give 12% I. The incorporation of 2 2,6-diaminopyridine units into the macrocyclic structure of I provides 6 complementary hydrogen bonds to barbituric acid derivs., resulting in a strong binding (Ks = 1.37 ı 106 M-1 for barbital) that is almost 100 fold greater than that (Ks = 2.08 104 ı M-1) to the acyclic analog II (R = PrCO).

IT **112817-60-4**
RL: PRP (Properties)
(binding affinity of, for barbiturates)

RN 112817-60-4 HCAPLUS
CN 1,3-Benzenedicarboxamide, N,N'-bis[6-[(1-oxobutyl)amino]-2-pyridinyl]- (9CI) (CA INDEX NAME)



L12 ANSWER 151 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

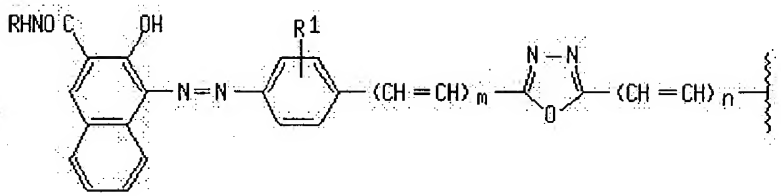
ACCESSION NUMBER: 1985:140808 HCAPLUS
DOCUMENT NUMBER: 102:140808
TITLE: Electrophotographic photoreceptor
PATENT ASSIGNEE(S): Mitsubishi Paper Mills, Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 13 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

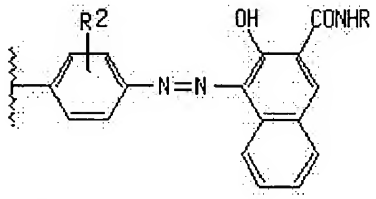
h eb c g cg b cg eb

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 59206841	A2	19841122	JP 1983-79656	19830507
JP 03000623	B4	19910108		

PRIORITY APPLN. INFO.: JP 1983-79656 19830507

GI





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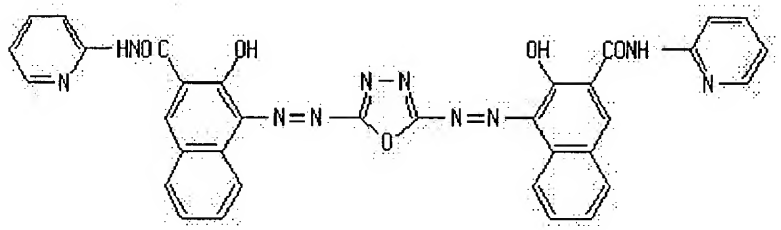


II

AB A photoreceptor for electrophotog. has a photosensitive layer contg. azo compd. having the general formula I (R = pyridyl, quinolyl, pyrimidyl; R1, R2 = H, lower alkyl, halo; m, n = 0, 1). These azo dyes provide high sensitivity and good charging behavior. The dyes are also stable to irradn. and heating. Thus, the dye II was synthesized as in the following: Ph 2-hydroxy-3-naphthoate 5 g was refluxed with 2-aminopyridine 2 g in PhNO3. The obtained coupler component 2-hydroxy-3-(N-2-pyridyl)naphthamide 2.5 g, and a tetrazolium salt 2.8 g obtained by diazotization of 2,5-di-(p-aminophenyl)-1,3,5-oxadiazole, were dissolved in EtOH and added to dil. aq. NaOH, to obtain crude II as purplish black crystals. Yield was 89% after purifn. An Al-laminated polyester film was coated with a butylamine soln. contg. II 0.5 and polyester resin (Vylon 200; Toyobo Co. Ltd.) 0.3 part to form a charge generating layer. A charge transfer layer was formed by coating a PhCl soln. contg. 4-N,N-diethylaminobenzaldehyde N,N-diphenylhydrazone 10 and resin U-100 (Unitica Ltd.). Obtained photoreceptor when charged to 1020 V showed a sensitivity (lx-s for half decay of voltage) of 2.8.

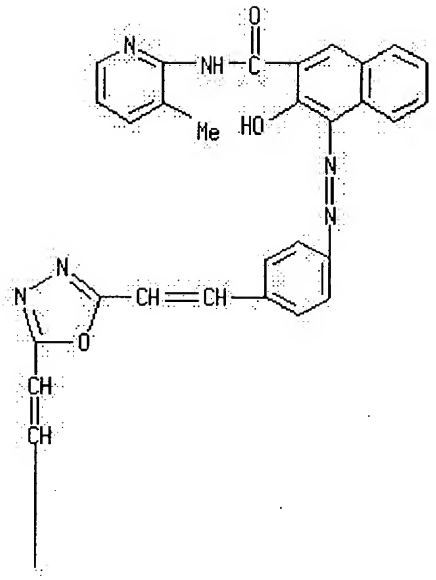
IT **95470-14-7**
RL: USES (Uses)
(electrophotog. charge generating agent)

RN 95470-14-7 HCAPLUS

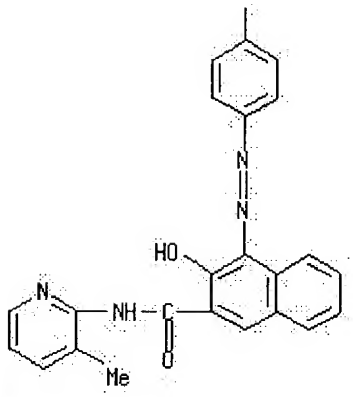
CN 2-Naphthalenecarboxamide, 4,4'-[1,3,4-oxadiazole-2,5-diylbis(2,1-ethenediyl-4,1-phenyleneazo)]bis[3-hydroxy-N-(3-methyl-2-pyridinyl)- (9CI) (CA INDEX NAME)

h eb c g cg b cg eb

PAGE 1-A



PAGE 2-A



L12 ANSWER 152 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 1976:123424 HCAPLUS
DOCUMENT NUMBER: 84:123424
TITLE: 4,4'-Stilbenebis-pyridooxazoles and related fluorescent whiteners and polymeric compositions whitened with them
INVENTOR(S): Crouse, Nathan N.
PATENT ASSIGNEE(S): Sterling Drug Inc., USA
SOURCE: U.S., 13 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3935195	A	19760127	US 1971-162620	19710714
US 3928228	A	19751223	US 1969-820005	19690428

h eb c g cg b cg eb

CA 982565	A1	19760127	CA 1970-81105	19700424
BE 749630	A	19701028	BE 1970-749630	19700428
CH 523885	A	19720615	CH 1970-523885	19700428
CH 523908	A	19720615	CH 1970-523908	19700428
CH 550818	A	19740628	CH 1971-13476	19700428
JP 48041005	B4	19731204	JP 1972-48678	19720518
CA 982566	A2	19760127	CA 1975-229517	19750617
CA 982590	A2	19760127	CA 1975-229491	19750617
PRIORITY APPLN. INFO.:			US 1969-820005	19690428
			CA 1970-81105	19700424

GI For diagram(s), see printed CA Issue.

AB Fluorescent whiteners (I, X = O, S, NH, NCH2CH2CN; A = pyridine residue) were prepd. and used to whiten polyester fibers. Thus, 4-HO2CC6H4CH:CHC6H4CO2H-4 [100-31-2] was added to polyphosphoric acid at 100°, the mixt. heated to 125°, 3-amino-4-pyridinol hydrochloride [58671-00-4] was added, the mixt. heated to 200° for 3.5 hr, and worked up to give I (X = O, orientation is oxazolo[4,5-c]pyridine) [29344-24-9]. The other I were similarly prepd.

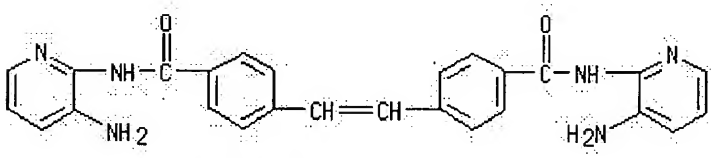
IT **34942-51-3P**

RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)

(prepn. and cyclization of)

RN 34942-51-3 HCAPLUS

CN Benzamide, 4,4'-(1,2-ethenediyl)bis[N-(3-amino-2-pyridinyl)- (9CI) (CA INDEX NAME)



L12 ANSWER 153 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 1975:593949 HCAPLUS

DOCUMENT NUMBER: 83:193949

TITLE: New aromatic polyamides. I. Polyamides from 4,4'-benzophenonedicarboxylic acid dichloride

AUTHOR(S): Guidotti, V.; Johnston, N. J.

CORPORATE SOURCE: Langley Res. Cent., NASA, Hampton, VA, USA

SOURCE: Polymer Preprints (American Chemical Society, Division of Polymer Chemistry) (1974), 15(1), 570-5
CODEN: ACPPAY; ISSN: 0032-3934

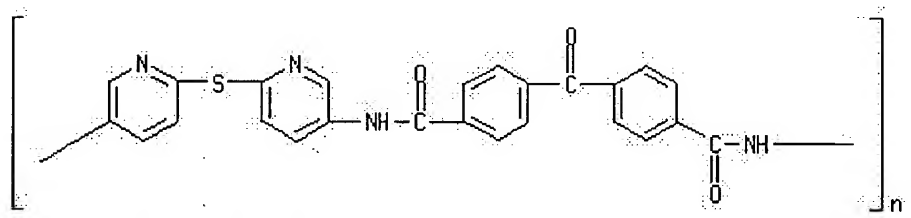
DOCUMENT TYPE: Journal

LANGUAGE: English

AB Thermogravimetric, thermochem., and soly. properties were detd. for 16-arom. polyamides made from 4,4'-benzophenonedicarbonyl chloride and diamines selected from the following 5 types: benzophenones, diphenylmethanes, diphenylsilyls, diarylsulfides, and compds. contg. 3 phenyl groups sepd. by methylene and/or carbonyl groups. Meta orientation in the amine moiety was very effective in decreasing glass temp. regardless of the nature of the flexible linking groups between the arom. rings. Diamines contg. meta and para linkages gave rise to polyamides with glass temps. closer to those from m,m'-isomers than to those originated by the p,p'-isomers. The dimethylsilyl group was the most effective linkage for lowering glass temp. An increase in the length of the repeat unit reduced glass temps. Nearly all of the polyamides had 2 addnl. regions of mech. loss below the glass temp.

h eb c g cg b cg eb

IT 57360-78-8
RL: USES (Uses)
(thermogravimetric, thermomech., and soly. properties of)
RN 57360-78-8 HCAPLUS
CN Poly(5,2-pyridinediylthio-2,5-pyridinediyliminocarbonyl-1,4-phenylenecarbonyl-1,4-phenylenecarbonylimino) (9CI) (CA INDEX NAME)



L12 ANSWER 154 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 1972:35235 HCAPLUS
DOCUMENT NUMBER: 76:35235
TITLE: Fluorescent whitening, heterocyclic-substituted stilbenes
INVENTOR(S): Crounse, Nathan N.
PATENT ASSIGNEE(S): Sterling Drug Inc.
SOURCE: Fr., 39 pp.
CODEN: FRXXAK
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

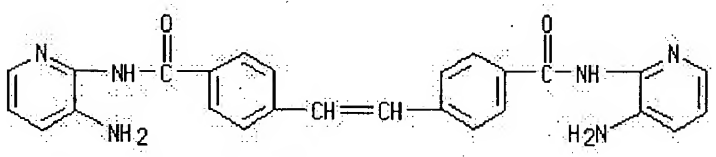
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 2046545	A5	19710305	FR 1970-15253	19700427
US 3928228	A	19751223	US 1969-820005	19690428
CA 982565	A1	19760127	CA 1970-81105	19700424
BE 749630	A	19701028	BE 1970-749630	19700428
CH 523885	A	19720615	CH 1970-523885	19700428
CH 523908	A	19720615	CH 1970-523908	19700428
CH 550818	A	19740628	CH 1971-13476	19700428
JP 48041005	B4	19731204	JP 1972-48678	19720518
CA 982566	A2	19760127	CA 1975-229517	19750617
CA 982590	A2	19760127	CA 1975-229491	19750617
PRIORITY APPLN. INFO.:			US 1969-820005	19690428
			CA 1970-81105	19700424

AB Oxazolo-, thiazolo-, and imidazopyridines (I, A represents a pyridine ring, X = O, S, NH, NCH2CH2CN), stable to heat and light and useful for fluorescent whitening poly(ethylene terephthalate) spin melts, were prepd. by cyclization of 4,4'-stilbenebiscarboxamides. For example, a mixt. of polyphosphoric acid and 4,4'-stilbenedicarboxylic acid was heated to 125.deg., 3-amino-4-pyridinol-HCl added, heated 3 hr at 200.deg., and the mixt. quenched in water to give 4,4'-bis(2-oxazolo[4,5-c]pyridyl)stilbene (II) [29344-24-9]. Five other I were similarly prepd. In an alternate method of prepn., 3-amino-2-chloropyridine was treated with p-MeC6H4COCl to give the amide which was heated in polyphosphoric acid to give 2-(p-tolyl)oxazolo[5,4-b]pyridine (III); heating III with S at 218-31.deg. for 10.5 hr gave 4,4'-bis(2-oxazolo[5,4-b]pyridyl)stilbene [27336-31-8].

IT 34942-51-3P

h eb c g cg b cg eb

RL: IMF (Industrial manufacture); PREP (Preparation)
(prepn. of)
RN 34942-51-3 HCAPLUS
CN Benzamide, 4,4'-(1,2-ethenediyl)bis[N-(3-amino-2-pyridinyl)- (9CI) (CA INDEX NAME)



L12 ANSWER 155 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 1971:499260 HCAPLUS
DOCUMENT NUMBER: 75:99260
TITLE: Fluorescent whiteners based on heterocyclic-substituted stilbenes
INVENTOR(S): Crounse, Nathan N.
PATENT ASSIGNEE(S): Sterling Drug Inc.
SOURCE: Ger. Offen., 43 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2020817	A	19710603	DE 1970-2020817	19700428
US 3928228	A	19751223	US 1969-820005	19690428
CA 982565	A1	19760127	CA 1970-81105	19700424
BE 749630	A	19701028	BE 1970-749630	19700428
CH 523885	A	19720615	CH 1970-523885	19700428
CH 523908	A	19720615	CH 1970-523908	19700428
CH 550818	A	19740628	CH 1971-13476	19700428
JP 48041005	B4	19731204	JP 1972-48678	19720518
CA 982566	A2	19760127	CA 1975-229517	19750617
CA 982590	A2	19760127	CA 1975-229491	19750617
PRIORITY APPLN. INFO.:			US 1969-820005	19690428
			CA 1970-81105	19700424

GI For diagram(s), see printed CA Issue.
AB Three 4,4'-bis(2-oxazolopyridinyl)-stilbenes (I, one of X, Y, and Z = N, others are CH) and two 4,4'-bis(imidazopyridin-2-yl)stilbenes (II, R = H or CH2CH2CN), heat- and light-stable fluorescent whiteners, esp. for poly(ethylene terephthalate), were prepd. For example, a mixt. of polyphosphoric acid and 4,4'-stilbenedicarboxylic acid was heated 3.5 hr with 3-amino-4-pyridinol-HCl at 200° to give 4,4'-bis(2-oxazolo[4,5-c]pyridinyl)stilbene (I, X = Z = CH, Y = N). Similarly prepd. was 4,4'-bis(2-oxazolo[5,4-b]pyridinyl)stilbene (I, X = N, Y, = Z = CH). Reaction of di-K 4,4'-stilbenedicarboxylate (III) with SOCl2 in PhCl gave the diacid chloride, which was treated with 2-amino-3-pyridinol in PhCl-C5H5N and then with aq. Na2CO3 to form N,N'-bis(3-hydroxy-2-pyridinyl)-4,4'-stilbenedicarboxamide (IV); IV was cyclized by heating with p-MeC6H4SO3H in C6H3Cl3 to form 4,4'-bis(2-oxazolo[4,5-b]pyridinyl)stilbene (I, X = Y = CH, Z = N). 4,4'-Bis(3H-imidazo[4,5-b]pyridin-2-yl)stilbene (II, R = H) (V) was similarly prepd. from III and 2,3-diaminopyridine. Reaction of V with acrylonitrile gave

h eb c g cg b cg eb

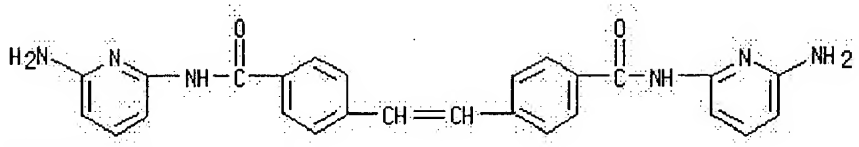
4,4'-bis[3-(2-cyanoethyl)-3H-imidazo[4,5-b]pyridin-2-yl]stilbene (II, R = CH2CH2CN).

IT **33761-32-9P**

RL: IMF (Industrial manufacture); PREP (Preparation)
(prepn. of)

RN 33761-32-9 HCAPLUS

CN 4,4'-Stilbenedicarboxamide, N,N'-bis(6-amino-2-pyridyl)- (8CI) (CA INDEX NAME)



L12 ANSWER 156 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 1969:449810 HCAPLUS

DOCUMENT NUMBER: 71:49810

TITLE: Syntheses and properties of 1H-pyrrolo[2,3-b] pyridines

AUTHOR(S): Herbert, R.; Wibberley, D. G.

CORPORATE SOURCE: Sch. Pharm., Sunderland Polytech., Sunderland, UK

SOURCE: Journal of the Chemical Society [Section] C: Organic (1969), (11), 1505-14
CODEN: JSOOAX; ISSN: 0022-4952

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 71:49810

GI For diagram(s), see printed CA Issue.

AB Five different routes for the prepn. of 1H-pyrrolo[2,3-b]pyridines (I) were investigated. A no. of 2-, 3-, and 4-alkyl and -aryl substituted derivs. were prepd. by two of these methods which involved modifications of Madelung- and Fischer-syntheses of indoles. I undergo nitration, nitrosation, bromination, iodination, and reaction with Mannich bases predominantly at the 3-position although one example of nitration at the 2-position was also found. Bis[3-(1H-pyrrolo[2,3-b]-pyridyl)]methanes are formed by reaction with aldehydes, and treatment of 2-phenyl-1H-pyrrolo[2,3-b]pyridine with nitrosobenzene yields 2-phenyl-3-phenylimino-3H-pyrrolo[2,3-b]pyridine. A further example of a deriv. of this isomeric 3H-system is 3-diazo-2-phenyl-3H-pyrrolo[2,3-b]pyridine which is formed from the corresponding amine by basification of the diazonium salt. 1-Substituted Grignard derivs. yield 3-iodo-compds. on treatment with H2O2 but only 1-acyl derivs. with acyl chlorides. Treatment of 2-phenyl-1H-pyrrolo[2,3-b]pyridine with CHCl3 and alkali caused ring-expansion to a 1,8-naphthyridine. A no. of unexpected products were isolated both in the syntheses of the 1H-pyrrolo[2,3-b]pyridines and in their reactions with electrophiles. Ir, N.M.R., and mass spectra were used to establish all structures.

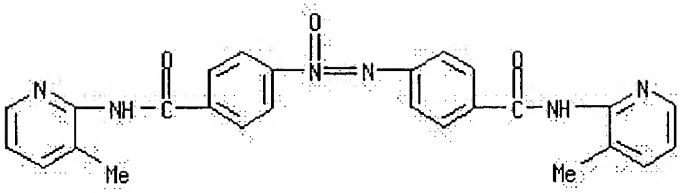
IT **23612-54-6P**

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 23612-54-6 HCAPLUS

CN Benzamide, 4,4'-azoxybis[N-(3-methyl-2-pyridyl)- (8CI) (CA INDEX NAME)

h eb c g cg b cg eb



L12 ANSWER 157 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 1969:57675 HCAPLUS
DOCUMENT NUMBER: 70:57675
TITLE: Substituted amino pyridines
INVENTOR(S): Thiele, Kurt; Von Bebenburg, Walter
PATENT ASSIGNEE(S): Deutsche Gold- und Silber-Scheideanstalt vorm. Roessler
SOURCE: S. African, 35 pp.
CODEN: SFXXAB
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
ZA 6702799		19680327	ZA	
DE 1670522			DE	
DE 1670523			DE	
FR 6877			FR	
GB 1191302			GB	
US 3481943		19690000	US	
US 3513171		19700000	US	
US 3712900		19730000	US	
US 3787429		19740000	US	
PRIORITY APPLN. INFO.:			DE	19660512

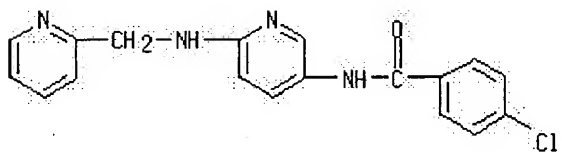
GI For diagram(s), see printed CA Issue.

AB 2-Chloro-5-nitropyridine (I) (80 g.) was added gradually to 110 g. PhCH2NH2 at 160°. After the exothermic reaction ceased, the mixt. was poured into H2O to give 82% 2-benzylamino-5-nitropyridine (II, R = R1 = H, R2 = Ph) (III), m. 133-4° (EtOH). 2-Amino-6-chloro-3-nitropyridine (IV) (69.6 g.) was added gradually to 172 g. PhCH2NH2 at 90°, the mixt. stirred at 100° 30 min. after the reaction ceased and dissolved in 1 l. Me2CO, and H2O added to incipient turbidity to give 94% II (R = NH2, R1 = H, R2 = Ph), m. 132°. Similarly prepd. and purified via its HCl salt was 81% dl-II (R = NH2, R1 = Me, R2 = Ph), m. 104-6°. A mixt. of 158 g. I, 108 g. 2-aminomethylpyridine, 1.5 l. iso-PrOH, and 138 g. K2CO3 was refluxed 7 hrs., cooled, and filtered, and the filtrate washed with H2O, dried, and evapd. to give 86.7% II (R = R1 = H, R2 = 2-pyridyl), m. 156-7°. IV (80 g.) was added gradually to a mixt. of 80 g. m-F3CC6H4CH2-NH2, 200 ml. PrOH, and 36.5 g. K2CO3 at 90° and the mixt. stirred 30 min. more and poured into H2O to ppt. 52% II (R = NH2, R1 = H, R2 = m-F3CC6H4), m. 105-8°. III (100 g.) and 30 g. Raney Ni in 500 ml. MeOH was hydrogenated at 50° 20 atm. to give 67% 2-benzylamino-5-aminopyridine (V, R = R1 = R2 = H, R3 = Ph) (VI), b0.2 180-5°. Similarly prepd. were the following V (R = H) [R1, R2, R3, % yield, m.p., b.p./mm., and m.p. of HCl salt (mono- or di-) given]: H, H, 2-pyridyl, 97, 100° (iso-PrOH), 210-28°/0.7, -; NH2, H, Ph, 65, 80-90°, -, 217-18° (mono); NH2, H, m-F3CC6H4, -, -, -, 205° (di); NH2, dl-Me, Ph, 68, -, -, 160-70° (di)

h eb c g cg b cg eb

(MeOH-Et2O); NH2, H, o-ClC6H4, -, -, -, 218° (di) (decompn.) (aq. EtOH). All V (R = H) were rapidly oxidized in air. VI (20 g.) treated with 10 g. Ac2O below 40° gave 13 g. V (R = Ac, R1 = R2 = H, R3 = Ph), m. 140-1° (MeOH). ClCO2Et (9.6 ml.) was added dropwise to 20 g. VI in 8.5 ml. C5H5N and 100 ml. Me2CO, the mixt. stirred 30 min. at room temp. and concd., the residue in C6H6 washed with H2O, the org. phase dried, C6H6 evapd., and the residue in MeOH treated with HCl/iso-PrOH to give 11 g. V.HCl (R = EtO2C, R1 = R2 = H, R3 = Ph), m. 145-6° (MeOH- Et2O). Other V were prepd. similarly, using Me2CO or dioxane as solvent (R, R1, R2, R3, % yield, m.p., and m.p. HCl salt given): EtO2C, H, H, 2-pyridyl, 21.4, -, 230° (EtOH-MeOH); EtCO, H, H, 2-pyridyl, 37, 126-7° (iso-PrOH), -; p-ClC6H4-CO, H, H, 2-pyridyl, 44, 187° (MeOH), -; EtO2C, NH2, H, Ph, -, -, 208-9° (EtOH); PrO2C, NH2, H, Ph, -, -, 225-30° (EtOH); CH2: CHCO, NH2, H, Ph, -, -, 230-5°; EtO2C, NH2, H, m-F3CC6H4, -, -, 213°; Ph(CH2)2O2C, NH2, H, m-F3CC6H4, -, -, 150-60° (aq. MeOH); CH2:CHCO, NH2, H, m-F3CC6H4, 42, -, 230-5°; EtCO, NH2, dl-Me, Ph, 42, -, 205-10° (H2O); EtO2C, NH2, dl-Me, Ph, 24, -, 155-7° (dioxane-Et2O); iso-PrO2C, NH2, H, Ph, -, -, 225-30° (decompn.). V were also prepd. by treating the filtered hydrogenation mixts. directly with the resp. reagents, without isolating the intermediate 3-aminopyridines (R, R1, R2, R3, and m.p. of HCl salt given): EtO2C, NH2, H, p-MeOC6H4, 202° (MeOH); tert-BuCO, NH2, H, p-MeOC6H4, 225-6°; EtO2C, NH2, H, p-ClC6H4, 219-20°; Ac, NH2, H, p-ClC6H4, 260° (decompn.); EtO2C, NH2, H, o-ClC6H4, 171°; EtCO, NH2, H, o-ClC6H4, 242-4° (H2O); CH2:CHCO, NH2, H, o-ClC6H4, 230-2° (decompn.); EtO2C, NH2, H, 3,4-CH2O2C6H3, 213°; EtCO, NH2, H, 3,4-CH2O2C6H3, 241°; EtO2C, NH2, H, p-MeC6H4, 208-9° (H2O); EtCO, NH2, H, p-MeC6H4, 268-9°; EtO2C, NH2, H, 2,4-Me2C6H3, 216-17°; EtO2C, NH2, H, 2,5-Me2C6H3, 217-18°; EtO2C, NH2, H, 3,4-Me2C6H3, 221°; EtCO, NH2, H, 3,4-Me2C6H3, 250° (decompn.); EtO2C, NH2, H, p-iso-PrC6H4, 217-18° (EtOH); EtCO, NH2, H, p-iso-PrC6H4, 242-51°; MeO2C, iso-PrNH, H, Ph, 187-8° (iso-PrOH-Et2O). V are pharmaceuticals with antiphlogistic and analgesic effects.

IT **21630-54-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 21630-54-6 HCAPLUS
CN Benzamide, p-chloro-N-[6-[(2-pyridylmethyl)amino]-3-pyridyl]- (8CI) (CA INDEX NAME)



L12 ANSWER 158 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 1965:463083 HCAPLUS
DOCUMENT NUMBER: 63:63083
ORIGINAL REFERENCE NO.: 63:11559b-c
TITLE: Pyrido[3,2-d]pyrimidin-4(3H)-ones
AUTHOR(S): Irwin, W. J.; Wibberley, D. G.
CORPORATE SOURCE: Tech. Coll., Sunderland, UK
SOURCE: Journal of the Chemical Society, Abstracts (1965),

h eb c g cg b cg eb

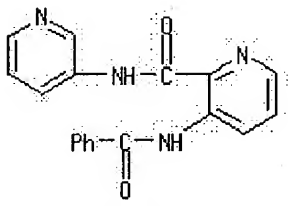
(Aug.), 4240-6
CODEN: JCSAAZ; ISSN: 0590-9791
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 63:63083

AB 2-Methyl- and 2-phenylpyrido[3,2-d][1,3]oxazin-4-ones are prepd. from 3-aminopicolinic acid. Treatment of these with primary amines yielded derivs. of 3-acetamido- and 3-benzamidopicolinamide, which were cyclized to give two series of 2,3-disubstituted pyrido[3,2-d]pyrimidin-4(3H)-ones.

IT **3295-45-2**, Picolinamide, 3-benzamido-N-3-pyridyl-
(prepn. of)

RN 3295-45-2 HCAPLUS

CN Picolinamide, 3-benzamido-N-3-pyridyl- (7CI, 8CI) (CA INDEX NAME)



L12 ANSWER 159 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 1965:463082 HCAPLUS
DOCUMENT NUMBER: 63:63082
ORIGINAL REFERENCE NO.: 63:11558g-h,11559a-b
TITLE: 2-Diethoxymethyl compounds in the 2-imidazoline and Δ2-tetrahydroypyrimidine series
AUTHOR(S): Baganz, Horst; Rabe, Siegfried; Repplinger, Joachim
CORPORATE SOURCE: Tech. Univ., Berlin
SOURCE: Chemische Berichte (1965), 98(8), 2572-5
CODEN: CHBEAM; ISSN: 0009-2940
DOCUMENT TYPE: Journal
LANGUAGE: German
OTHER SOURCE(S): CASREACT 63:63082

GI For diagram(s), see printed CA Issue.

AB I (R = Bu) (II), I (R = PhCH2) (III), and IV were prepd. On acid hydrolysis the 2,4-dinitrophenyl-hydrazones of the aldehydes but not the free aldehydes could be isolated. (EtO)2CHCO2Et (V) (35.2 g.) and 23.2 g. BuNHCH2CH2NH2 heated with 3 drops concd. HCl under a column with the continuous removal of the EtOH formed, and the residual mixt. heated then during 6 hrs. to 200° yielded 28.8 g. II, b0.1 75°, n25D 1.4569. II (2.3 g.) and 2.0 g. 2,4-(O2N)2C6H3NHNH2 (VI) in 5 cc. concd. H2SO4 and 20 cc. 50% EtOH heated 3 hrs. on a water bath gave 2.7 g. 2,4-dinitrophenylhydrazone sulfate of 1-butyl-2-imidazoline-1-carboxaldehyde (VII), m. 238° (EtOH). V (35.2 g.) and 30.0 g. PhCH2NHCH2CH2NH2 (VIII) gave similarly 35.2 g. III, b0.1 142°, n25D 1.4569; picrate m. 118° (EtOH). III (2.6 g.) and 2.0 g. VI in concd. HCl refluxed 5 hrs. gave 0.45 g. 2,4-dinitrophenylhydrazone hydrochloride of the 1-PhCH2 analog of VII, m. 251° (aq. EtOH). V (44 g.) and 125 g. H2N(CH2)3NH2 refluxed 72 hrs. gave 38 g. IV, b0.1 88°, n25D 1.4748. IV (5.0 g.) and 5.0 g. VI in 150 cc. EtOH and 50 cc. 20% HCl heated 3 hrs. on a water bath gave 7.2 g. 2,4-dinitrophenylhydrazone hydrochloride of Δ2-tetrahydropyrimidine-2-carboxaldehyde, m. 283° (aq. EtOH). III (13.1 g.) and 50 cc. 15% HCl refluxed 35 hrs. gave 74% CO2 and 7.7 g. VIII.2HCl, m. 243° (aq. EtOH). II (11.4 g.) and 50 cc. 40% H2SO4 refluxed 6 hrs. gave 62%

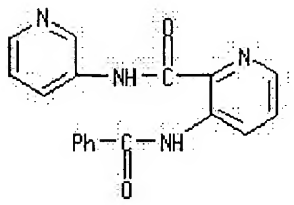
h eb c g cg b cg eb

CO2, 11% CO, and 7.8% HCO2H. IV (5.0 g.) and 25% H2SO4 heated 48 hrs. gave 41% CO2 and 37% CO.

IT **3295-45-2**, Picolinamide, 3-benzamido-N-3-pyridyl-
(prepn. of)

RN 3295-45-2 HCAPLUS

CN Picolinamide, 3-benzamido-N-3-pyridyl- (7CI, 8CI) (CA INDEX NAME)



L12 ANSWER 160 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 1961:144175 HCAPLUS
DOCUMENT NUMBER: 55:144175
ORIGINAL REFERENCE NO.: 55:27306e-i,27307a
TITLE: Reductive cleavage of 2,6-diacyldiamino-2-butoxy-3,5'-azopyridines
AUTHOR(S): Melandri, Marcello; Vittorina, Gerosa; Buttini, Annibale
CORPORATE SOURCE: Soc. ital. prodotti Schering, Milan
SOURCE: Annali di Chimica (Rome, Italy) (1960), 50, 125-33
CODEN: ANCRAI; ISSN: 0003-4592
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

AB Attempts to prep. 2,6-diacyldiamino-3-aminopyridines by the reductive cleavage of the azo linkage in the above cited structure gave rise to secondary reactions. The course of the reaction was influenced by the reducing agent, solvent, and acyl group. Treating 2,6-diamino-2'-butoxy-3,5'-azopyridine (I) with glacial AcOH gave yellowish-orange 2,6-diacetyldiamino-2'-butoxy-3,5'-azopyridine, m. 190-1° (decompn.). I and BzCl in C5H5N gave yellow 2,6-dibenzoyldiamino-2'-butoxy-3,5'-azopyridine (II), m. 170-1° (decompn.). I and maleic anhydride in C6H6 afforded brown 2,6-dimaleyldiamino-2'-butoxy-3,5'-azopyridine, m. 145-7° (decompn.), and fusion of I with o-C6H4(CO)2O gave reddish-orange 2,6-diphthaloyldiamino-2'-butoxy-3,5'-azopyridine (III), m. 233-5°. A suspension of 0.01 mole III in 50 cc. of 15% HCl was heated on a H2O-bath while 5 g. pulverized Fe was added in small amts. Heating was terminated after the orange color of III disappeared and the reaction product was basified with 20% NaOH and the filtrate continuously extd. with Et2O to remove 2,5-BuO(H2N)C5H3N. Neutralizing the basic layer gave 2,6,3-(NH2)2(OH)C5H2N (IV) which changed rapidly to the quinone as indicated by its blue color. Filtering through a sintered disk and copious washing with H2O gave the quinone of IV, m. >300°. Reducing II gave 2-phenyl-5-benzoylamino-3H-pyrido[2,3-b]imidazole (V), m. 261-3° (70% EtOH), λ 227 and 331, E1%1 610 and 930. V loses H2O of hydration at 115-20°. Heating V several hrs. at 180-90° caused crystal modification, m. 205-6°. During the redn. of V, its tendency to saponify at the amide linkage with the formation of the amine hydrochloride was avoided by interrupting the reaction at the opportune time and by filtering off V. It was purified by boiling in 5% NaOH to remove any Fe and its hydrate, followed by acidifying the filtrate and washing the ppt. with H2O. A suspension of 0.01 g.-mole III in 80 cc. glacial AcOH was heated 30 min.

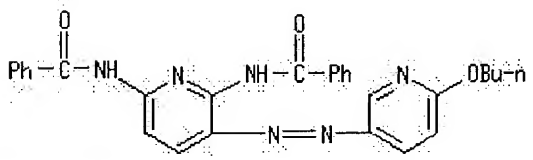
h eb c g cg b cg eb

on the H2O bath while adding Fe in small amts., the wt. of which corresponded to about half of III. Cooling and removing any excess Fe and its acetate was followed by pouring the filtrate into 100 cc. boiling H2O. Cooling gave 2-butoxy-5-phthaloylaminopyridine, m. 163-4° (several times from 95% EtOH). Evapg. the filtrate in vacuo, taking up the residue in dil. HCl, filtering, and neutralizing gave an unidentified product, m. 170°. Similar redn. of II gave V. Subjecting III to redn. with N2H4.H2O in the presence of 10% Pd-C gave phthalylhydrazide, m. 340-3°. II was recovered unchanged when treated similarly.

IT **123885-77-8**, Pyridine, 2,6-dibenzamido-6'-butoxy-3,3'-azodi- (prepn. of)

RN 123885-77-8 HCAPLUS

CN Pyridine, 2,6-dibenzamido-6'-butoxy-3,3'-azodi- (6CI) (CA INDEX NAME)



L12 ANSWER 161 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 1957:81498 HCAPLUS

DOCUMENT NUMBER: 51:81498

ORIGINAL REFERENCE NO.: 51:14738f-i,14739a-e

TITLE: Sulfur-containing pyridine derivatives. LIII. Smiles rearrangement in pyridine derivatives and syntheses of azaphenothiazine derivatives. 1

AUTHOR(S): Maki, Yoshifumi

CORPORATE SOURCE: Univ. Kyoto

SOURCE: Yakugaku Zasshi (1957), 77, 485-90
CODEN: YKKZAJ; ISSN: 0031-6903

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

AB 6,2,3-Cl(HS)(H2N)C5H2N (0.5 g.), in 10 ml. MeOH contg. 0.3 g. KOH and 0.5 g. 2-ClC6H4NO2 in a sealed tube heated 5 hrs. at 100°, the product concd., and recrystd. from MeOH gave 0.15 g. 6,2,3-Cl(2-O2NC6H4S)(H2N)C5H2N (IX), cubes, m. 181°; 3-AcNH analog (X) of IX, m. 155°. X (0.12 g.) in 5 ml. dil. MeOH and 0.02 g. KOH treated with excess MeI, kept until the soln. turned neutral, the solvent removed, and the residue recrystd. from MeOH gave 0.08 g. 6,2,3-Cl-(MeS)(2-O2NC6H4NAc)C5H2N, cubes, m. 162-3°. Heating of X 15 min. at 100° and the product recrystd. from MeOH gave 6,2,3-Cl(MeS)(2-O2NC6H4NH)C5H2N, needles, m. 182-3°. 6,3,2-Cl(MeNH)(RS)C5H2N (R = 5-nitro-2-pyridyl) (0.2 g.) in dil. MeOH and 0.05 g. KOH refluxed 10 min., cooled, let stand with the excess MeI, the product concd., and recrystd. from MeOH gave 0.1 g. 6,2,3-Cl(MeS)(RMeN)C5H2N, cubes, m. 119°. 6,2,3-Cl(RS)(R1CONH)C5H2N (XI) (R1 = Me) (XIa) m. 170-1°; XI (R1 = Ph) m. 197-8°; XI (R1 = p-O2NC6H4) m. 186-7°. XI (0.2 g.) in dil. MeOH and 0.05 g. KOH stirred, the soln. treated with the excess MeI and the product recrystd. from EtOH gave 0.2 g. 6,2,3-Cl(MeS)(RNH)C5H2N, m. 184°. XIa in EtOH contg. AcONa heated 20 min. and the product recrystd. from EtOH gave 6,2,3-Cl(MeS)(RAcN)C5H2N, m. 151-2°. Similarly, 6,2,3-Cl(RSO2)(AcNH)C5H2N (XII) gave 6,2,3-Cl(MeSO2)(RNH)C5H2N (XIII), m. 212°. 6,2,3-Cl(MeS)(RNH)C5H2N (0.1 g.) in 10 ml. AcOH treated portionwise with 0.07 g. KMnO4, stirred 1.5 hrs., the excess KMnO4 and MnO2 decompd. with H2O2, and the product

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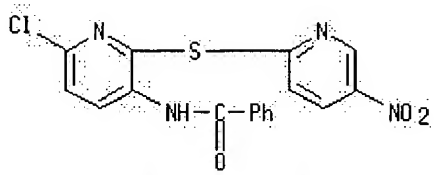
recrystd. from dil. MeOH gave 0.1 g. XIII, m. 212°. XII (0.2 g.) in 5 ml. dil. MeOH and 0.05 g. KOH refluxed for formation of 6,2,3-Cl(HO3S)(RNH)C5H2N, the soln. poured into 5 ml. H2O contg. 0.45 g. HgCl2, the product filtered off, refluxed 1 hr. with 10 ml. EtOH and 10 ml. HCl, the EtOH removed and the residue extd. with AcOEt gave 0.05 g. 6,3-Cl(RNH)C5H3N (XIV), m. 264-5° (decompn.). 2,5-Cl(H2N)C5H3N (0.3 g.) and 0.37 g. 2,5-Cl(O2N)C5H3N heated 1 hr. at 120° gave 0.1 g. XIV, m. 264-5° (decompn.). 6,2,3-Cl(HS)(H2N)C5H2N (XVa) (0.5 g.) in MeOH contg. 0.2 g. KOH and 0.6 g. 1,3,4-Cl2(O2N)C6H3 in EtOH let stand 2 hrs., the soln. filtered, the filtrate concd., and the residue recrystd. from MeOH gave 0.3 g. 6,2,3-Cl[4,2-Cl-(O2N)C6H3S](H2N)C5H2N (XV), plates, m. 159°; 3-AcNH analog (XVI), needles, m. 147°. XVI gave a transition product in 2 hrs. at room temp.; this treated with MeI and the product recrystd. from AcOEt gave C12H9O2N3Cl2S, needles, m. 220°. XVa (0.3 g.) in MeOH contg. 0.15 g. KOH and 0.3 g. 2,3-Cl(O2N)C5H3N let stand 1 hr. and the product recrystd. from AcOEt gave 0.15 g. 6,2,3-Cl(R2S)(H2N)C5H2N (XVII) (R2 = 3-nitro-2-pyridyl), needles, m. 183°; 3-AcNH analog (XVIII) of XVII, needles, m. 173°. XVIII (0.1 g.) in 6-7 ml. EtOH and 0.02 g. KOH refluxed 15 min., the EtOH removed, the residue extd. with AcOEt, the AcOEt removed, and the residue recrystd. from EtOH gave 0.05 g. 7-chloro-10H-dipyrido[2,3-b; 3,2-e]-1,4-thiazine, needles, m. 249° (decompn.). Similarly, 0.5 g. XVa, MeOH contg. 0.35 g. KOH and 0.6 g. 4,3-Cl(O2N)C5H3N gave 0.6 g. 6,2,3-Cl(R3S)(H2N)C5H2N (XIX) (R3 = 3-nitro-4-pyridyl), m. 219° (decompn.); 3-AcNH analog (XX) of XIX, m. 230-1° (decompn.). Heat-transition of XX and treating the product with MeI gave 2-MeS deriv., C11H7O2N4ClS, needles, m. 228-9° (from dioxane.). XVa (0.5 g.) in 3 ml. C5H5N, 2 ml. H2O, and 3 ml. MeOH treated with 0.62 g. 1,2,4-Cl(O2N)2C6H3 in MeOH, H2O added, the ppt. filtered off, and recrystd. from MeOH gave 0.6 g. 6,2,3-Cl[2,4-(O2N)2C6H3S](H2N)C5H2N (XXI), needles, m. 193-4°; 3-AcNH analog (XXII) of XXI, plates, m. 204°. XXI and XXII yielded a transition product, C12H9O4N4ClS, needles, m. 212°. Me2CO (50 ml.), 0.3 g. KOH, and 10 ml. 95% EtOH while refluxing, treated with 1 g. XXII, refluxed 15 min., the solvent removed, and the residue recrystd. from EtOH gave 0.5 g. 2-chloro-8-nitro-5H-benzo[b]pyrido[3,2-e]-1,4-thiazine (XXIII), needles, m. 225°. XVa (0.5 g.) in 5 ml. EtOH treated with 0.8 g picryl chloride, the product filtered off, and recrystd from AcOEt gave 0.2 g. 6,8-di-NO2 analog of XXIII, dark purple needles, m. 260° (decompn.).

IT **101439-38-7**, Pyridine, 3-benzamido-6-chloro-5'-nitro-2,2'-thiodi-
(prepn. of)

RN 101439-38-7 HCAPLUS

CN Pyridine, 3-benzamido-6-chloro-5'-nitro-2,2'-thiodi- (6CI) (CA INDEX NAME)



L12 ANSWER 162 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 1957:25524 HCAPLUS

DOCUMENT NUMBER: 51:25524

ORIGINAL REFERENCE NO.: 51:5068c-i,5069a-d

h eb c g cg b cg eb

TITLE: Search for trypanocides. III. Analogs of suramin
AUTHOR(S): Adams, A.; Ashley, J. N.; Bader, H.
CORPORATE SOURCE: May & Baker Ltd., Dagenham, UK
SOURCE: Journal of the Chemical Society, Abstracts (1956) 3739-44
CODEN: JCSAAZ; ISSN: 0590-9791
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

AB cf. C.A. 51, 4375i. Some symmetrical ureas which were based on the structure of suramin (I) but contained thiazol-2-yl, 2-pyridyl, 5-sulfo-2-pyridyl, and 4-carboxy-3-hydroxyphenyl groups instead of the naphthalenetrisulfonic acid group were synthesized. All of the compds. were inactive against Trypanosoma congolense and T. rhodesiense infections in mice. 4-Methyl-3-nitrobenzoyl chloride (II) (21 g.) added slowly to a cooled soln. of 10.5 g. 2-aminothiazole in C5H5N, then heated 10 min. on the steam bath, and purified gave 24.3 g. 2-(4-methyl-3-nitrobenzamido)thiazole (III), plates, m. 192° (from alc.). 4-Aminosalicylic acid (IV) (153 g.) and 100 g. II in Me2CO refluxed 1 hr. gave 146 g. 4-(4-methyl-3-nitrobenzamido) salicylic acid (V), white needles, m. 264-5° (decompn.), violet color with FeCl3, slightly sol. in hot 2N Na2CO3 from which the Na salt crystd. in fine needles, m. above 300°. A suspension of 105.2 g. III in 2 l. AcOH was hydrogenated at room temp. and atm. pressure in the presence of Adams catalyst during 20 hrs. to give 76.8 g. 2-(3-amino-4-methylbenzamido)thiazole (VI), needles, m. 208°. m-Nitrobenzoyl chloride (VII) and VI similarly yielded 94% 2-(4-methyl-3-m-nitrobenzamidobenzamido)-thiazole (VIIa), m. 283-5° (from aq. C5H5N). p-(3-Amino-4-methylbenzamido)salicylic acid (VIII) (143 g.) and 93 g. VII refluxed 3 hrs. in Me2CO and the product stirred 1 hr. with 2N NaOH and kept overnight, the mixt. filtered, the filtrate dild. with alc. and acidified gave 108 g. 4-(4-methyl-3-m-nitrobenzamidobenzamido)salicyli c acid, prisms, m. 271-2° (decompn.). 2-(3-Aminobenzamido-4-methylbenzamido)thiazole (IX) (11.6 g.) in AcOH treated with 11.6 g. NaOAc.3H2O in H2O, then a slow stream of COCl2 passed in, and after 0.5 hr. the mixt. poured into H2O and kept overnight, the product dissolved in C5H5N, refluxed with C, and crystd. gave 6.8 g. 1,3-bis(3-m-benzamido-4-methylbenzamido)urea (X), m. 305-7° (from aq. C5H5N or aq. AcOH). m-Nitrobenzenesulfonyl chloride (28.5 g.) heated 1 hr. with 30 g. VI in C5H5N yielded 2-(4-methyl-3-m-nitrobenzenesulfonamidobenzamido)thiazole, needles, m. 215-17°. The following compds. were prepd. by methods similar to those recorded above. Analogs, 3,4-RNHXC6H3(NO2)Me, of IV were prepd. (substituents at X and R, crystn. form, % yield, and m.p. given): CO, 2-pyridyl, plates, 96, 152-3°; CO, 5-sulfo-2-pyridyl, needles, 78, 316° (decompn.). Analogs, 3,4-RNHXC6H3(NH2)Me, of VI were prepd. (substituents X and R, crystn. form, % yield, and m.p. given): CO, 2-pyridyl, rectangular prisms, 64, 182.5-3.0°; CO, 5-sulfo-2-pyridyl, needles, 70, 306°; CO, 4-carboxy-3-hydroxyphenyl, fawn prisms, 91, 251°. Analogs, m-ZXC6H4NO2(Z = 2,5-Me(RNHCO)C6H3NH), of VIIa were prepd. (substituents X and R, crystn. state, % yield, and m.p. given): CO, 2-pyridyl, needles, 90, 228.5°; SO2, 2-pyridyl, yellow prisms, 90, 192-3°; CO, 5-sulfo-2-pyridyl, colorless, 74, 312°; SO2, 5-sulfo-2-pyridyl, plates, 44, 223°. The amino-amide analogs, m-ZXC6H4NH2, of IX were prepd. (substituents X and R, crystn. state, % yield, and m.p. given): CO, thiazol-2-yl, needles, 90, 270.0-70.5°; SO2, 2-thiazolyl, fawn prisms, 94, 287-9°; CO, 2-pyridyl, needles, 90, 217°; SO2, 2-pyridyl, needles, 80, 206-7°; CO, 5-sulfo-2-pyridyl, cream-colored, 74, 287°; SO2, 5-sulfo-2-pyridyl, colorless, 83, 240-50°; CO, 4-carboxy-3-hydroxyphenyl, fawn prisms, 50, 243-4°. The analogs, (m-ZXC6H4NH)2CO, of X were prepd.

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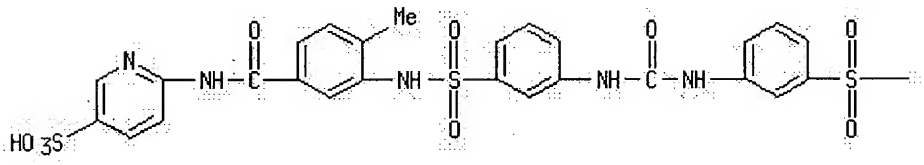
(substituents X and R, crystn. state, % yield, and m.p. given): SO2, 2-thiazolyl, yellow prisms, 70, 240-5°; CO, 2-pyridyl, needles, 53, 266°; SO2, 2-pyridyl, cream-colored, 60, 220°; CO, 5-sulfo-2-pyridyl, cream-colored, 91, 300° (decompn.); SO2, 5-sulfo-2-pyridyl, cream-colored, 84, slowly darkens above 295°; CO, 4-carboxy-3-hydroxyphenyl, pale brown, 65, 250-3°. II (15.5 g.) shaken 1 hr. with 11.9 g. IV in 200 cc. 3% aq. NaOH, the solid filtered off, washed with H2O, and dried, then stirred 10 min. with 50 cc. N NaOH, and AcOH added gave 2.9 g. 4-methyl-3-nitrobenzoic acid (XI), m. 190°. The residue gave 5.9 g. solids which were recrystd. to give O,N-bis(4-methyl-3-nitrobenzoyl)-m-aminophenol (XII), m. 167-8°, then resolidified and rem. 191°, gave no color with FeCl3, did not couple with β-naphthol, or decomp. aq. Na2CO2. The filtrate from the original reaction was acidified and afforded 7.7 g. of the salt of IV and 4-methyl-3-nitrobenzoic acid (XIII), prisms, m. 165° (decompn.), acid to litmus, liberated CO2 from aq. NaHCO3, violet color with FeCl3, and red after diazotization and coupling with β-naphthol. Na 4-aminosalicylate (XIV) (2.11 g.) in 10 cc. H2O added to 1.81 g. 4-methyl-3-nitrobenzoic acid in 10 cc. N NaOH, and the mixt. acidified gave 3.2 g. XIII (from PhMe). XIV dihydrate (10 g.) in 2N NaOH and Me2CO treated with COCl2 as above gave 83% 1,3-bis(3-hydroxy-4-carboxyphenyl)urea. Similarly the Na salt of 4-(3-amino-4-methylbenzamido)salicylic acid gave the analogous urea in 80% yield, needles, m. 289-90° (decompn.).

IT **108625-65-6**, 3-Pyridinesulfonic acid, 6,6'-{ureylenebis[m-phenylenesulfonylimino(4-methyl-m-phenylene)carbonylimino]}di-
(prepn. of)

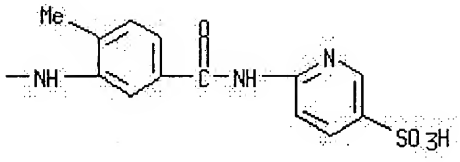
RN 108625-65-6 HCAPLUS

CN 3-Pyridinesulfonic acid, 6,6'-[ureylenebis[m-phenylenesulfonylimino(4-methyl-m-phenylene)carbonylimino]]di- (6CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B



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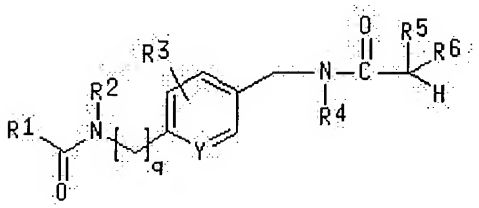
L12 ANSWER 1 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | More References

ACCESSION NUMBER: 2004:550938 HCAPLUS
DOCUMENT NUMBER: 141:106380
TITLE: Preparation of amide-substituted (hetero)aryl derivatives as inhibitors of microsomal triglyceride transfer protein (MTP) and apolipoprotein B (Apo B) secretion
INVENTOR(S): Bertinato, Peter; Maddux, Todd Michael
PATENT ASSIGNEE(S): Pfizer Products Inc., USA
SOURCE: PCT Int. Appl., 80 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004056775	A1	20040708	WO 2003-IB5982	20031210
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2004132779	A1	20040708	US 2003-742199	20031219
PRIORITY APPLN. INFO.:			US 2002-435378P	P 20021220

OTHER SOURCE(S): MARPAT 141:106380
GI



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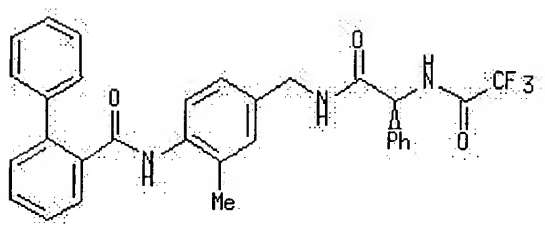


II

h eb c g cg b cg eb

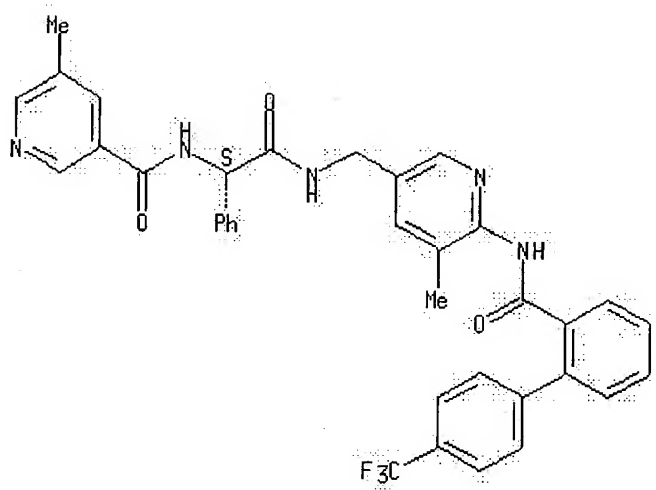
AB Title compds. I [R1 = substituted (hetero)aryl; R2 = H, (cyclo)alkyl, acyl, etc.; q = 0-1; R3 = H, halo, alkyl, haloalkyl, etc.; Y = substituted alkyl, N; R4 = H, (cyclo)alkyl, acyl, etc.; R5 = alkyl, Ph, heteroaryl; R6 = H, alkyl, etc.] are prepd. For instance, 4'-trifluoromethylbiphenyl-2-carboxylic acid N-(5-aminomethyl-3-methylpyridin-2-yl)amide (prepn. given) is coupled to (S)-N-(Boc)phenylglycine (CH2Cl2, DCC, i-Pr2NEt) and subsequently treated with TFA/PyBOP/i-Pr2NEt to give II. I are inhibitors of microsomal triglyceride transfer protein (MTP) and/or apolipoprotein B (Apo B) secretion; they are useful for the treatment of obesity and related diseases, as well as prevention and treatment of atherosclerosis and its clin. sequelae, for lowering serum lipids and in the prevention and treatment of related diseases.

IT 719299-78-2P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of amide-substituted (hetero)aryl derivs. as inhibitors of microsomal triglyceride transfer protein (MTP) and apolipoprotein B (Apo B) secretion)

RN 719299-78-2 HCAPLUS

CN 3-Pyridinecarboxamide, 5-methyl-N-[(1S)-2-[[[5-methyl-6-[[[4'-(trifluoromethyl)[1,1'-biphenyl]-2-yl]carbonyl]amino]-3-pyridinyl]methyl]amino]-2-oxo-1-phenylethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 2 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | CHIPT References

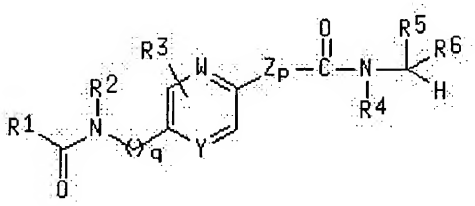
ACCESSION NUMBER: 2004:546481 HCAPLUS
DOCUMENT NUMBER: 141:106375
TITLE: Preparation of amide-substituted (hetero)aryl derivatives as inhibitors of microsomal triglyceride transfer protein (MTP) and apolipoprotein B (Apo B) secretion
INVENTOR(S): Bertinato, Peter; Bronk, Brian Scott; Cheng, Hengmiao; Chang, George; Cole, Bridget McCarthy; Li, Jin; Ruggeri, Roger Benjamin
PATENT ASSIGNEE(S): Pfizer Products Inc., USA
SOURCE: PCT Int. Appl., 90 pp.

h eb c g cg b cg eb

CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004056777	A1	20040708	WO 2003-IB5809	20031208
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2004132745	A1	20040708	US 2003-742197	20031219
PRIORITY APPLN. INFO.:			US 2002-435377P	P 20021220

OTHER SOURCE(S): MARPAT 141:106375
GI



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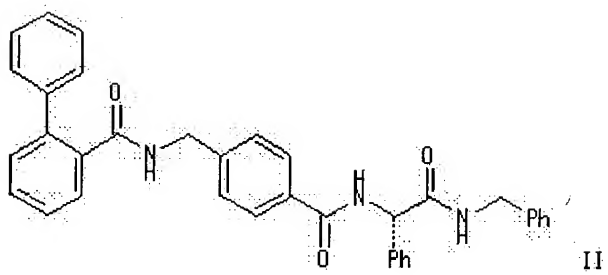


II

AB Title compds. I [R1 = substituted (hetero)aryl; R2 = H, (cyclo)alkyl, acyl, etc.; p, q = 0-1; R3 = H, halo, alkyl, haloalkyl, etc.; Y, W = substituted alkyl, N, etc.; Z = SCH2, CH2, OCH2; R4 = H, (cyclo)alkyl, acyl, etc.; R5 = alkyl, Ph, heteroaryl; R6 = H, alkyl, etc.] are prepd. For instance, 4-[[(4'-trifluoromethylbiphenyl-2-carbonyl)amino]methyl]benzoic acid Me ester (prepn. given) is sapond. and coupled to (S)-N-benzyl-2-amino-2-phenylacetamide hydrochloride. (CH2Cl2, i-Pr2NEt, PyBOP) to give II. I are inhibitors of microsomal triglyceride transfer protein (MTP) and/or apolipoprotein B (Apo B) secretion; they are useful for the treatment of obesity and related diseases, as well as prevention and treatment of atherosclerosis and its clin. sequelae, for lowering serum lipids and in the prevention and treatment of related diseases.

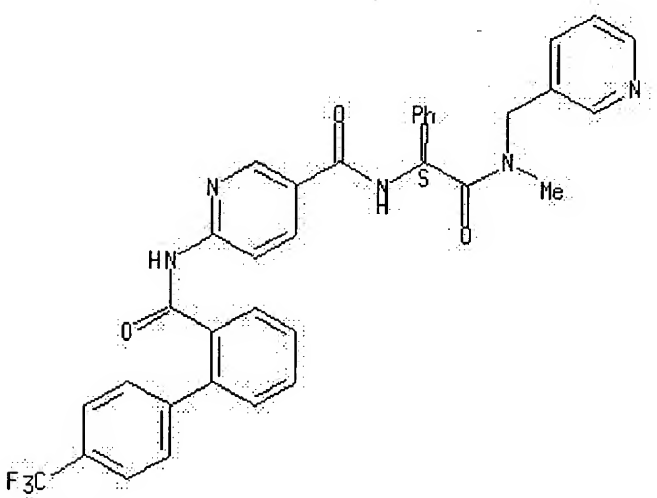
IT **720682-98-4P**

h eb c g cg b cg eb

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of amide-substituted (hetero)aryl derivs. as inhibitors of microsomal triglyceride transfer protein (MTP) and apolipoprotein B (Apo B) secretion)

RN 720682-98-4 HCAPLUS
CN 3-Pyridinecarboxamide, N-[(1S)-2-[methyl(3-pyridinylmethyl)amino]-2-oxo-1-phenylethyl]-6-[[[4'-(trifluoromethyl)[1,1'-biphenyl]-2-yl]carbonyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 3 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 2004:546480 HCAPLUS
DOCUMENT NUMBER: 141:89019
TITLE: Substituted biphenyl-4-carboxylic acid arylamide analogues as VR1 receptors modulators
INVENTOR(S): Bakthavatchalam, Rajagopal; Blum, Charles A.; Brielmann, Harry; Darrow, James W.; De Lombaert, Stephane; Yoon, Taeyoung; Zheng, Xiaozhang
PATENT ASSIGNEE(S): Neurogen Corporation, USA
SOURCE: PCT Int. Appl., 170 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

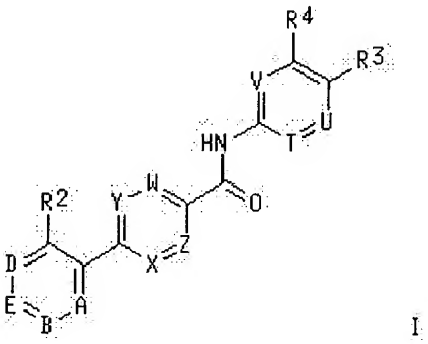
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004056774	A2	20040708	WO 2003-US40878	20031219

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ, BY,

h eb c g cg b cg eb

KG, KZ, MD, RU
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: US 2002-435118P P 20021219
OTHER SOURCE(S): MARPAT 141:89019
GI



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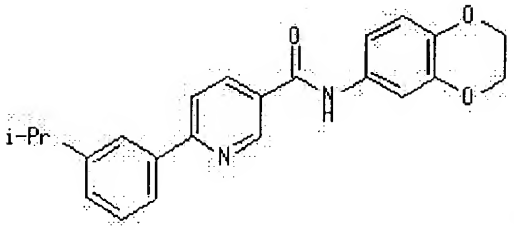


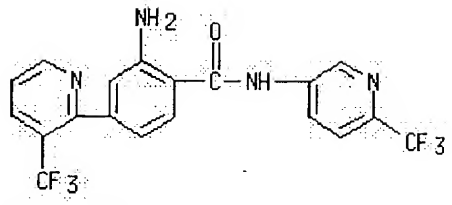
II

AB The title compds. [such as I; A, B, D, E, W, X, Y, Z = CR1, N; T, U, V = CR8, N; R1 = halo, CN, NO2, etc.; R2 = NO2, CN, NHOH, etc.; R3, R4 = H, halo, alkyl, etc.; R8 = H, halo, OH, etc.] which are capable of modulating capsaicin receptor activity (biol. data given), are provided. E.g., the nicotinamide II was prepd. starting from 3-isopropylphenylboronic acid, Me 6-chloronicotinate and 2,3-dihydrobenzo[1,4]dioxin-6-ylamine. Such ligands may be used to modulate receptor activity in vivo or in vitro, and are particularly useful in the treatment of pain and other conditions assocd. with receptor activation in humans, domesticated companion animals and livestock animals. Pharmaceutical compns. and methods for treating such disorders are provided, as are methods for using such ligands for receptor localization studies.

IT **717111-52-9P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of substituted biphenyl-4-carboxylic acid arylamide analogs as VR1 receptors modulators for treating pain assocd. with various conditions)

RN 717111-52-9 HCAPLUS
CN Benzamide, 2-amino-4-[3-(trifluoromethyl)-2-pyridinyl]-N-[6-(trifluoromethyl)-3-pyridinyl]- (9CI) (CA INDEX NAME)

h eb c g cg b cg eb



L12 ANSWER 4 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Cited References

ACCESSION NUMBER: 2004:390239 HCAPLUS
DOCUMENT NUMBER: 140:406743
TITLE: Preparation of aryl and heteroaryl amides, in particular benzamides and pyridinyl amides, as apolipoprotein B (Apo B) secretion inhibitors
INVENTOR(S): Inoue, Yoshikazu; Terasawa, Takeshi; Takasugi, Hisashi; Nagayoshi, Akira; Ueshima, Koji; Sawada, Masae; Furukawa, Yoshiro; Mikami, Masafumi; Hinoue, Kazumasa; Fukumoto, Daisuke
PATENT ASSIGNEE(S): Fujisawa Pharmaceutical Co., Ltd., Japan; Daiso Co., Ltd.; et al.
SOURCE: PCT Int. Appl., 331 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004039795	A2	20040513	WO 2003-JP13683	20031027
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2004133008	A1	20040708	US 2003-694091	20031028
PRIORITY APPLN. INFO.:			AU 2002-952331 A	20021029
			AU 2003-902622 A	20030527

OTHER SOURCE(S): MARPAT 140:406743
GI

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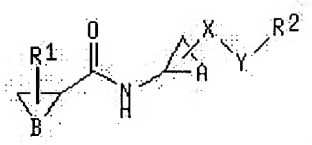

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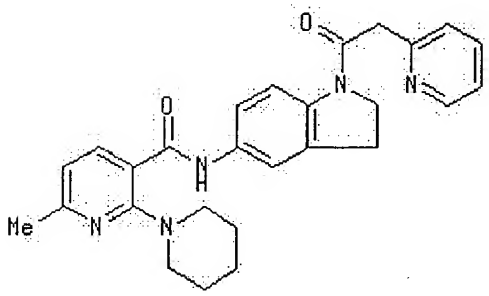


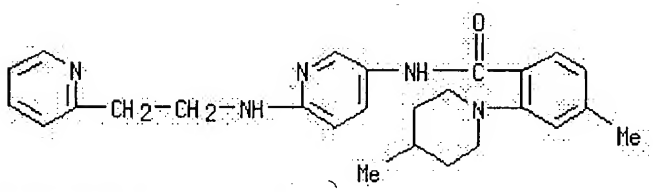
II

AB Title compds. I [wherein R1 = H, lower alk/en/yl, halo(lower)alkyl, cyclo(lower)alkyl, lower alkoxy, lower alkylthio, acyl, NH2 and derivs., (un)substituted aryl; R2 = H, (un)substituted hetero/aryl; X = a bond or bivalent residue derived from piperazine; Y is -(A1)n-(A2)m-; A1 = O, NH, CO, NHCO, CONH, CH2CONH, etc.; A2 = (un)substituted lower alkylene, n and m = independently 0 or 1; A = bivalent residue derived from hetero/arene; B = bivalent residue derived from (un)substituted hetero/arene; and their salts] were prepd. as inhibitors of apolipoprotein B (Apo B) secretion, and as a medicament for prophylactic and treatment of diseases or conditions resulting from elevated circulating levels of Apo B. For example, II was prepd. by acylation of N-(2,3-dihydro-1H-indol-5-yl)-6-methyl-2-(1-piperidinyl)nicotinamide (prepn. given) with 2-pyridinyl acetic acid dihydrochloride. N-[4-[[2-(6-Amino-2-pyridinyl)ethyl]amino]phenyl]-4-chloro-2-(dimethylamino)benzamide (III) displayed 85.9% inhibition of Apo B secretion at 10-8 M,. III, at a dose of 0.32 mg/kg lowered lipid levels in ddY-mice by 52% after 2 h. I are useful as hypolipemic, antidiabetic, and cardiovascular agents.

IT **689151-32-4P**, 4-Methyl-2-(4-methyl-1-piperidinyl)-N-[6-[[2-(2-pyridinyl)ethyl]amino]-3-pyridinyl]benzamide
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(Apo B inhibitor; prepn. of amides as apolipoprotein B secretion inhibitors)

RN 689151-32-4 HCAPLUS

CN Benzamide, 4-methyl-2-(4-methyl-1-piperidinyl)-N-[6-[[2-(2-pyridinyl)ethyl]amino]-3-pyridinyl]- (9CI) (CA INDEX NAME)



L12 ANSWER 5 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 2004:368213 HCAPLUS
DOCUMENT NUMBER: 141:106807
TITLE: Multiple recognition of barbiturate guests by

h eb c g cg b cg eb

	Hamilton-receptor-functionalized dendrimers
AUTHOR(S):	Dirksen, Anouk; Hahn, Uwe; Schwanke, Frank; Nieger, Martin; Reek, Joost N. H.; Voegtle, Fritz; De Cola, Luisa
CORPORATE SOURCE:	Institute of Molecular Chemistry, Universiteit van Amsterdam, Amsterdam, 1018 WV, Neth.
SOURCE:	Chemistry--A European Journal (2004), 10(8), 2036-2047 CODEN: CEUJED; ISSN: 0947-6539
PUBLISHER:	Wiley-VCH Verlag GmbH & Co. KGaA
DOCUMENT TYPE:	Journal
LANGUAGE:	English

AB The well-known unsubstituted "Hamilton receptor" was mono-functionalized with an amino group and attached at the periphery of poly(propyleneamine) dendrimers through the use of an activated ester. Four generations of Hamilton-receptor-functionalized dendrimers (HR-dendrimers) were synthesized and characterized by 1H and 13C NMR spectroscopy and MALDI-TOF mass spectrometry. The photophys. properties of the HR-dendrimers were investigated by UV/Vis as well as with steady-state and time-resolved fluorescence spectroscopy. The dendrimers were used as multivalent hosts for the barbiturate guests Barbital (I) and [Re(Br)(CO)3(barbi-bpy)] (II; barbi-bpy = 5-[4-(4'-methyl)- 2,2'-bipyridyl]methyl-2,4,6-(1H,3H,5H)-pyrimidinetrione). The stable adducts formed between the dendritic architectures (the hosts) and the barbiturate guests I and II were investigated by 1H NMR spectroscopy and photophys. methods. The binding consts. of the barbiturate guests for binding to ref. compd. N,N'-bis-[6-(3,3-dimethylbutyrylamino)pyridin-2-yl]-5-octanoylaminoisophthalamide (III; with a single receptor unit) in chloroform were found to be 1.4 103 ǀM-1 and 1.5 105 ǀM-1 for 7 and 8, resp. Binding of I to the dendrimers enhances the weak emission of the Hamilton receptor. This increase in emission is also generation dependent; it was found to be most pronounced in the case of III and the least in the case of the fourth-generation dendrimer. The unexpected increase in the quantum yield of emission from the HR-dendrimers with increasing generation could be caused by the rather rigid conformation of the Hamilton receptors in later-generation compds., which is a result of intramol. aggregation and steric hindrance at the periphery of the dendrimer. The photoinduced energy transfer from the excited state of the HR-dendrimers to the lower-lying excited state of the guest II was used to probe the formation of host-guest complexes. The rate of energy transfer was calcd. to be 3.6 1010 ǀS-1. Energy transfer in the host-guest complex of III with II only occurred in the presence of a strong base, which shows that the basic amine core in the HR-dendrimers is crucial for this photoinduced process. The binding of II to the dendrimers is completely reversible: II can be exchanged with a competitive guest such as I and the emission of the HR-dendrimer is restored.

IT **717111-21-2P**

RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. and host-guest complexes for model N,N'-bis[(dimethylbutyrylamino)pyridinyl]octanoylaminoisophthalamide)

RN 717111-21-2 HCAPLUS

CN 1,3-Benzenedicarboxamide, N,N'-bis[6-[(3,3-dimethyl-1-oxobutyl)amino]-2-pyridinyl]-5-[(1-oxooctyl)amino]- (9CI) (CA INDEX NAME)

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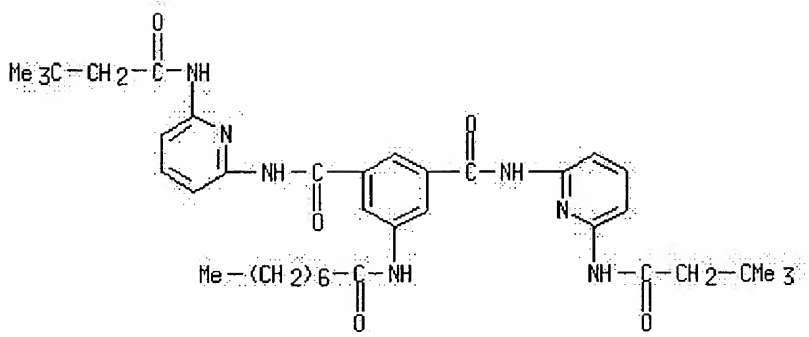
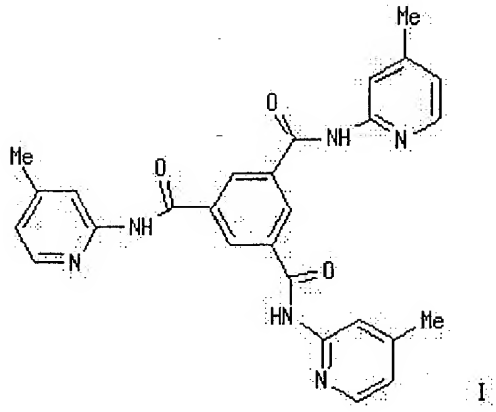


REFERENCE COUNT: 71 THERE ARE 71 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 6 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 2004:245051 HCAPLUS
DOCUMENT NUMBER: 140:423878
TITLE: Pyridine-based receptors with high affinity for carbohydrates. Influence of the degree of steric hindrance at pyridine nitrogen on the binding mode
AUTHOR(S): Mazik, Monika; Sicking, Willi
CORPORATE SOURCE: Institut fuer Organische Chemie der Technischen Universitaet Braunschweig, Braunschweig, 38106, Germany
SOURCE: Tetrahedron Letters (2004), 45(15), 3117-3121
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

AB Remarkable changes in the binding affinity and selectivity of pyridine-based receptors, e.g. I, toward glycosides have been obsd. when the degree of steric hindrance at pyridine nitrogen atom decreases. Crystal structure of I is reported.

IT **692731-95-6P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (of pyridine-based receptors with high affinity for carbohydrates and influence of degree of steric hindrance at pyridine nitrogen on binding mode)

RN 692731-95-6 HCAPLUS

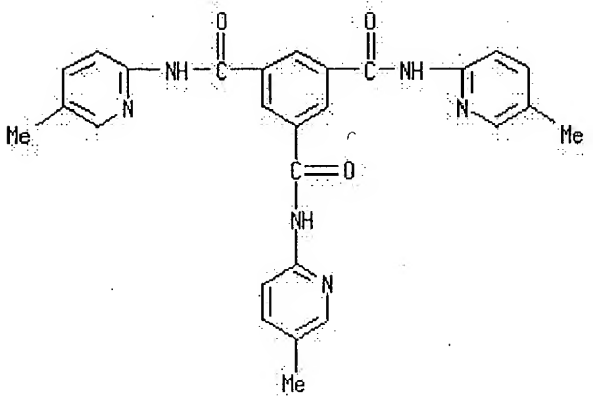
CN α-D-Glucopyranoside, methyl, compd. with N,N',N''-tris(5-methyl-2-

h eb c g cg b cg eb

pyridinyl)-1,3,5-benzenetricarboxamide (1:1) (9CI) (CA INDEX NAME)

CM 1

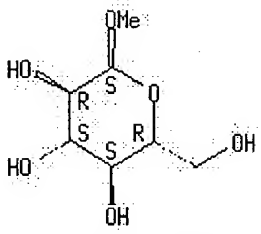
CRN 692731-93-4
CMF C27 H24 N6 O3



CM 2

CRN 97-30-3
CMF C7 H14 O6

Absolute stereochemistry. Rotation (+).



REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 7 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 2004:158446 HCAPLUS
DOCUMENT NUMBER: 140:331809
TITLE: Comparing the Quality and Predictiveness between 3D QSAR Models Obtained from Manual and Automated Alignment
AUTHOR(S): Tervo, Anu J.; Nyroenen, Tommi H.; Roenkkoe, Toni; Poso, Antti
CORPORATE SOURCE: Department of Pharmaceutical Chemistry, University of Kuopio, Kuopio, 70211, Finland
SOURCE: Journal of Chemical Information and Computer Sciences (2004), 44(3), 807-816
CODEN: JCISD8; ISSN: 0095-2338
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A set of 113 flexible cyclic urea inhibitors of human immunodeficiency virus protease (HIV-1 PR) was used to compare the quality and predictive

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power of CoMFA and CoMSIA models for manually or automatically aligned inhibitor set. Inhibitors that were aligned automatically with mol. docking were in agreement with information obtained from existing x-ray structures. Both alignment methods produced statistically significant CoMFA and CoMSIA models, with the best q2 value being 0.649 and the best predictive r2 being 0.754. The manual alignment gave statistically higher values, whereas the automated alignment gave more robust models for predicting the activities of an external inhibitor set. Both models utilized similar amino acids in the HIV-1 PR active site, supporting the idea that hydrogen bonds form between an inhibitor and the backbone carbonyl oxygens of Gly48 and Gly48' and also the backbone NH group of Asp30, Gly48, Asp29', and Gly48' of the enzyme. These results suggest that an automated inhibitor alignment can yield predictive 3D QSAR models that are well comparable to manual methods. Thus, an automated alignment method in creating 3D QSAR models is encouraging when a well-characterized structure of the target protein is available.

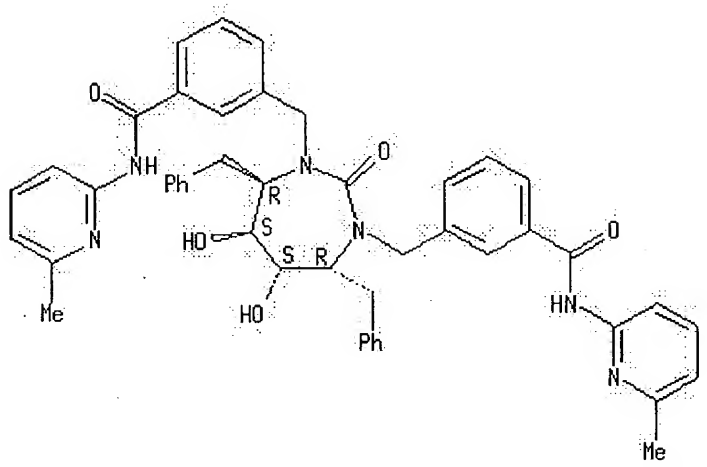
IT **183854-97-9**

RL: PAC (Pharmacological activity); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(comparing the quality and predictability between 3D QSAR CoMFA and CoMSIA models obtained from manual and automated alignment using cyclic urea HIV-1 virus protease inhibitors)

RN 183854-97-9 HCAPLUS

CN Benzamide, 3,3'-[[(4R,5S,6S,7R)-tetrahydro-5,6-dihydroxy-2-oxo-4,7-bis(phenylmethyl)-1H-1,3-diazepine-1,3(2H)-diyl]bis(methylene)]bis[N-(6-methyl-2-pyridinyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 49 THERE ARE 49 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 8 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

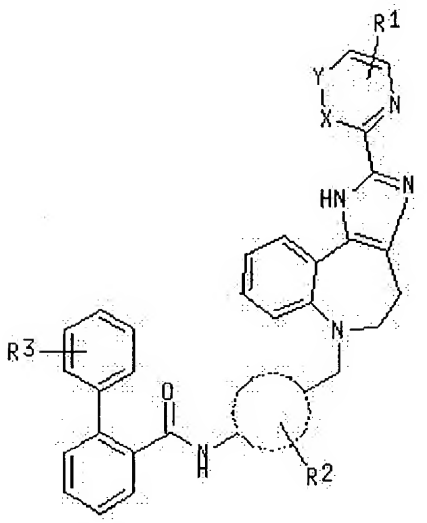
ACCESSION NUMBER: 2004:117842 HCAPLUS
DOCUMENT NUMBER: 140:152009
TITLE: Arginine vasopressin receptor antagonists containing 1,4,5,6-tetrahydroimidazo[4,5-d]benzazepine derivatives
INVENTOR(S): Koshio, Hiroyuki; Kakefuda, Akio; Sato, Ippei; Wakayama, Ryutaro; Sanagi, Masanao
PATENT ASSIGNEE(S): Yamanouchi Pharmaceutical Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 29 pp.

h eb c g cg b cg eb

CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2004043456	A2	20040212	JP 2003-141799	20030520
PRIORITY APPLN. INFO.:			JP 2002-149935 A	20020524

OTHER SOURCE(S): MARPAT 140:152009
GI



I

AB The invention provide pharmaceutical compds. I (ring D = phenylene, etc.; X,Y = CH, N; R1, R2, R3 = H, OH, halo, lower alkyl) as arginine vasopressin receptor antagonists, suitable for treatment of cardiac failure and hyponatremia. A compd. N-[4-[2-(2-pyridyl)-1,4,5,6-tetrahydroimidazo[4,5-d][1]benzazepine-6-carbonyl]phenyl]biphenyl-2-carboxamide (II) hydrochloride was prepd. The compd. showed antagonistic effect on V1A and V2 receptors without inhibiting CYP3A4 enzyme in in vitro assay. An injection compn. contg. II 1 mg/mL was formulated.

IT **433263-38-8P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(arginine vasopressin receptor inhibitors contg. 1,4,5,6-tetrahydroimidazo[4,5-d]benzazepine derivs.)

RN 433263-38-8 HCAPLUS
CN [1,1'-Biphenyl]-2-carboxamide, N-[5-[[4,5-dihydro-2-(2-pyridinyl)imidazo[4,5-d][1]benzazepin-6(1H)-yl]carbonyl]-2-pyridinyl]-, monohydrochloride (9CI) (CA INDEX NAME)

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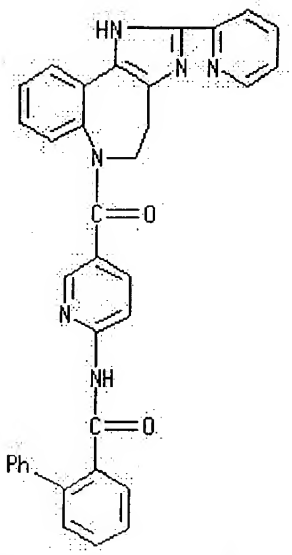

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L12 ANSWER 9 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 2004:105138 HCAPLUS
DOCUMENT NUMBER: 140:287798
TITLE: Synthesis and Analysis of Telechelic Polyisobutylenes for Hydrogen-Bonded Supramolecular Pseudo-Block Copolymers
AUTHOR(S): Binder, Wolfgang H.; Kunz, Michael J.; Kluger, Christian; Hayn, Getraud; Saf, Robert
CORPORATE SOURCE: Institute of Applied Synthetic Chemistry, Vienna University of Technology, Vienna, A-1060, Austria
SOURCE: Macromolecules (2004), 37(5), 1749-1759
CODEN: MAMOBX; ISSN: 0024-9297
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB New telechelic polyisobutylenes (PIB) with hydrogen-bonding motifs were prepd. Nucleobases such as thymine, uracil, and cytosine as well as chelate-type hydrogen-bonding donor-acceptors were affixed onto the end groups of the PIB. Starting with PIB of defined mol. wt., prepd. by living cationic polymn., hydroxy-terminated PIB was generated, which subsequently was transformed into the corresponding chloromethyl ether. Reaction with silylated nucleobases furnished the final nucleobase-telechelic PIB in high yields. The chelate-type PIB was prepd. by a sequence of nucleophilic/addn. reaction steps adapted to the low soly. of PIB polymers in polar solvents. The structure of the PIB polymers was proven by 1H NMR, 13C NMR, and MALDI-TOF MS anal. proving the complete conversion between the reaction steps in quant. yields. The pure PIB polymers with specific hydrogen bonding patterns will allow the investigation of supramol. pseudo-block copolymers.

IT **676267-93-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(model compd.; prepn. of model compds. for synthesis and anal. of telechelic polyisobutylenes for hydrogen-bonded supramol. pseudo-block copolymers)

RN 676267-93-9 HCAPLUS
CN 1,3-Benzenedicarboxamide, 5,5'-[1,6-hexanediylbis(oxy)]bis[N,N'-bis[6-[(1-oxobutyl)amino]-2-pyridinyl]- (9CI) (CA INDEX NAME)

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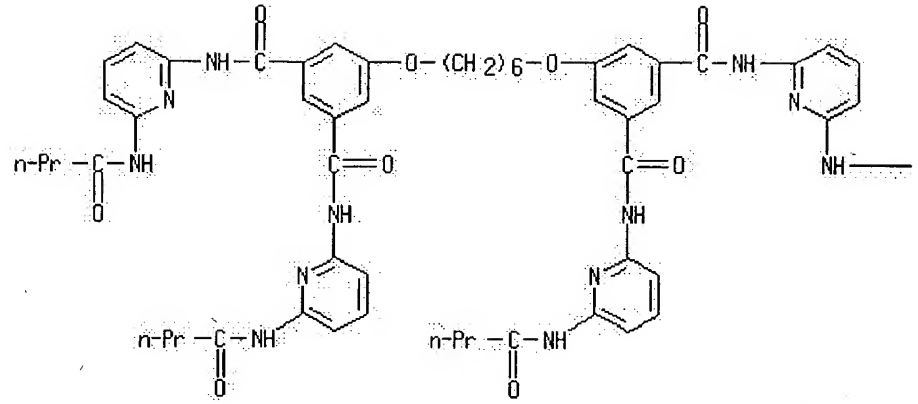
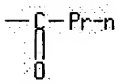
PAGE 1-A



PAGE 1-B



REFERENCE COUNT: 52 THERE ARE 52 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 10 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 2004:99292 HCAPLUS
DOCUMENT NUMBER: 140:321217
TITLE: Design, synthesis, and SAR of anthranilamide-based factor Xa inhibitors incorporating substituted biphenyl P4 motifs
AUTHOR(S): Zhang, Penglie; Bao, Liang; Zuckett, Jingmei F.; Goldman, Erick A.; Jia, Zhaozhong J.; Arfsten, Ann; Edwards, Susan; Sinha, Uma; Hutchaleelaha, Athiwat; Park, Gary; Lambing, Joseph L.; Hollenbach, Stanley J.; Scarborough, Robert M.; Zhu, Bing-Yan
CORPORATE SOURCE: Millennium Pharmaceuticals, Inc., Francisco, CA, 94080, USA
SOURCE: Bioorganic & Medicinal Chemistry Letters (2004), 14(4), 983-987
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

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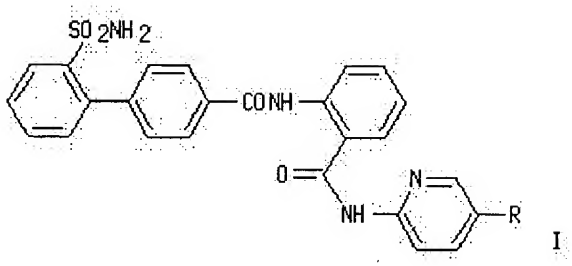


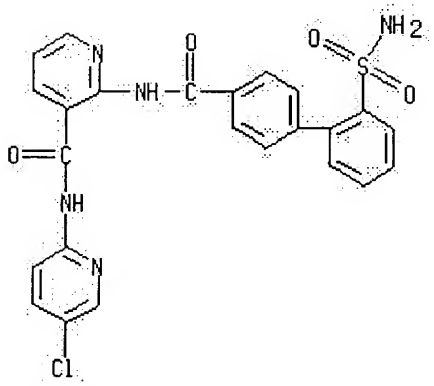
I

AB Anthranilamides I [R = Br, Cl] were designed and synthesized as selective and orally bioavailable factor Xa inhibitors. Structural modifications aimed at lowering their lipophilicity were performed at the central Ph ring and at the S4 binding biphenyl region by incorporating water solubilizing substituents. The resulting compds. are highly potent in vitro, and show improved activity in human plasma-based thrombin generation assay.

IT **330939-75-8P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(prepn. and structure-activity relationships of biphenylcarbamoylanthranilamides as factor Xa inhibitors)

RN 330939-75-8 HCAPLUS

CN 3-Pyridinecarboxamide, 2-[[[2'-(aminosulfonyl)[1,1'-biphenyl]-4-yl]carbonyl]amino]-N-(5-chloro-2-pyridinyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 11 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 2004:41463 HCAPLUS
DOCUMENT NUMBER: 140:77161
TITLE: Preparation of pyrimidinylaminobenzamides as inhibitors of protein kinases, in particular tyrosine kinases for treating neoplasm, especially leukemia
INVENTOR(S): Breitenstein, Werner; Furet, Pascal; Jacob, Sandra; Manley, Paul William
PATENT ASSIGNEE(S): Novartis A.-G., Switz.; Novartis Pharma G.m.b.H.
SOURCE: PCT Int. Appl., 83 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

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PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004005281	A1	20040115	WO 2003-EP7198	20030704
WO 2004005281	C1	20040506		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LT, LU, LV, MA, MD, MK, MN, MX, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SE, SG, SK, SY, TJ, TM, TN, TR, TT, UA, US, UZ, VC, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR

PRIORITY APPLN. INFO.: GB 2002-15676 A 20020705
GB 2002-29893 A 20021220

OTHER SOURCE(S): MARPAT 140:77161

GI

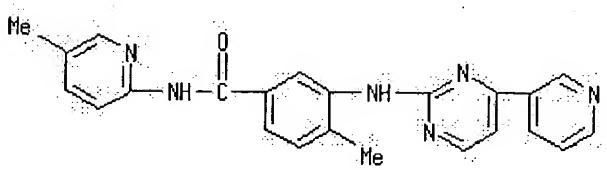
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Title compds. I [wherein R1 = H, alkoxy/carboxy/alkoxycarbonyl/phenyl/alkyl; R2 = H, (un)substituted cyclo/benzcyclo/alkyl, heterocyclyl, aryl, mono- or bicyclic heteroaryl; R1R2 = (un)substituted alkylene with 4-6 C atoms, benzalkylene with 4 or 5 C atoms, oxaalkylene with one O and 3 or 4 C atoms, azaalkylene with one N and 3 or 4 C atoms where N is (un)substituted by phenyl/alkoxycarbonyl/carboxy/carbamoyl/alkyl, alkoxycarbonyl, carboxy, (un)substituted Ph, pyridyl, pyrimidinyl, pyrazinyl, etc.; R4 = H, alkyl, halo; their N-oxides, tautomers, and pharmaceutical acceptable salts] were prepd. as inhibitors of protein kinases, in particular tyrosine kinases for treating neoplastic diseases, esp. leukemia. II was prepd. by amidation of 4-Methyl-3-[[4-(3-pyridinyl)-2-pyrimidinyl]amino]benzoic acid (prepn. given) with N,N-diethyl-1,3-benzenediamine in the presence of propylphosphonic anhydride/TEA/DMF at room temp. for 24 h. In an in vitro test, II inhibited C-Abl, KDR, and Flt3 tyrosine kinase in 98%, 88%, and 41% resp. I exhibited IC50 values for the inhibition of Flt-1 VEGF receptor tyrosine kinase in the range of 1-10,000 nM, preferably in the range of 1-100 nM. Thus, I and their pharmaceutical compns. are useful for treatment of neoplasm, in particular leukemia.

IT **641570-54-9P**, 4-Methyl-N-(5-methyl-2-pyridinyl)-3-[[4-(3-pyridinyl)-2-pyrimidinyl]amino]benzamide
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(tyrosine kinases inhibitor; prepn. of pyrimidinylaminobenzamides as inhibitors of tyrosine kinases in particular tyrosine kinases for treatment of leukemia)

RN 641570-54-9 HCAPLUS

CN Benzamide, 4-methyl-N-(5-methyl-2-pyridinyl)-3-[[4-(3-pyridinyl)-2-pyrimidinyl]amino]- (9CI) (CA INDEX NAME)



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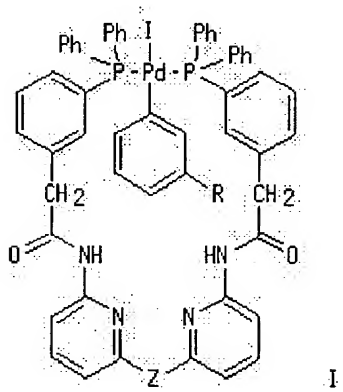
REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 12 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | CHNG References

ACCESSION NUMBER: 2004:37118 HCAPLUS
DOCUMENT NUMBER: 141:7245
TITLE: Preparation of a novel diphosphine-palladium macrocyclic complex possessing a molecular recognition site. Oxidative addition studies
AUTHOR(S): Larsen, Jens; Rasmussen, Brian S.; Hazell, Rita G.; Skrydstrup, Troels
CORPORATE SOURCE: Department of Chemistry and the Interdisciplinary Nanoscience Center, University of Aarhus, Aarhus C, 8000, Den.
SOURCE: Chemical Communications (Cambridge, United Kingdom) (2004), (2), 202-203
CODEN: CHCOFS; ISSN: 1359-7345
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 141:7245
GI



I

AB Macrocyclic diphosphine ligands having Hamilton's barbiturate binding domain interact with Pd(dba)2 giving mixt. of Pd(0) species; oxidative addn. reactions of aryliodide-substituted barbiturate gave trans-arylpalladium iodide complex featuring host-guest interactions of the barbiturate moiety with the macrocycle. Oxidative addn. of the substituted barbiturate, 3-IC6H4R (4, R = 5-methyl-2,4,6(1H,3H,5H)-pyrimidinetrion-5-ylmethyl) afforded complex I (6, Z = N,N'-isophthalimido), crystal structure of which revealed the hydrogen bonding between the barbiturate moiety and the macrocycle. Palladium(II) mol. assoc. I·[5-(3-butenyl)-5-methyl-2,4,6(1H,3H,5H)-pyrimidinetrione] (7; Z = N,N'-isophthalimido, R = H) in which the Ph group is directed to the outside of the macrocycle, was prepd. by oxidative addn. of iodobenzene in the presence of the substituted barbiturate. Crystal structure of 6 and 7 is described.

IT **112817-57-9**
RL: RCT (Reactant); RACT (Reactant or reagent)
(acylation; prepn. of palladium host-guest complexes of trans-macrocyclic diphosphine contg. Hamilton's barbiturate binding site)

RN 112817-57-9 HCAPLUS

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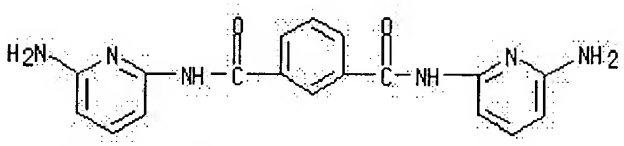
CN 1,3-Benzenedicarboxamide, N,N'-bis(6-amino-2-pyridinyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 13 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Other References

ACCESSION NUMBER: 2004:15636 HCAPLUS
DOCUMENT NUMBER: 140:217490
TITLE: Structural studies on hydrogen-bonding receptors for barbiturate guests that use metal ions as allosteric inhibitors
AUTHOR(S): Al-sayah, Mohammad H.; McDonald, Robert; Branda, Neil R.
CORPORATE SOURCE: Department of Chemistry, University of Alberta, Edmonton, AB, T6G 2G2, Can.
SOURCE: European Journal of Organic Chemistry (2004), (1), 173-182
CODEN: EJOCFK; ISSN: 1434-193X
PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 140:217490
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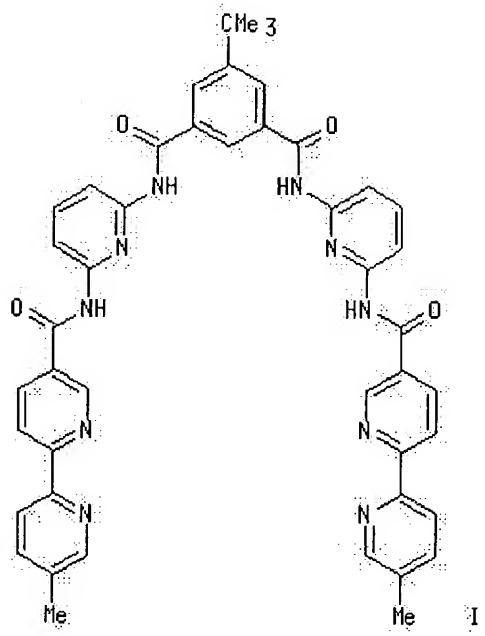

I

AB N,N'-bis(arylcarbonylaminopyridinyl)isophthalamides such as I are prepd. as barbiturate receptors in which the binding of barbiturate is regulated allosterically through the presence or absence of a metal capable of binding to the terminal aryl moieties. An N,N'-

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bis(arylcarbonylaminopyridinyl)isophthalamide with a terminal 2,2'-bipyridine-6-carbonyl moiety is prepd. and found incapable of binding 5,5-dibutylbarbituric acid; synthesis of other N,N'-bis(arylcarbonylaminopyridinyl)isophthalamides indicates that the lack of binding is caused by the presence of an intramol. hydrogen bond which disrupts the hydrogen bonds needed for binding of substrate. Modified receptor I (with terminal 2,2'-bipyridine-5-carbonyl moieties rather than 2,2'-bipyridine-6-carbonyl moieties) successfully binds 5,5-dibutylbarbituric acid with a Ka value of 2.8 103 ı M-1. I does not bind 5,5-dibutylbarbituric acid in the presence of zinc (II) triflate; the structure of the zinc complex of I is detd. by two-dimensional 1H NMR expts. The structure of one of the N,N'-bis(arylcarbonylaminopyridinyl)isophthalamides is detd. by X-ray crystallog.

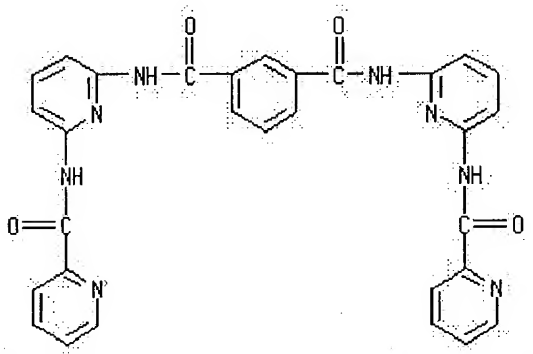
IT **665026-34-6P**

RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)

(crystal structure; prepn. of N,N'-bis(arylcarbonylaminopyridinyl)isophthalamides as hydrogen-bonding receptors for barbituric acids regulated allosterically by the presence or absence of zinc)

RN 665026-34-6 HCAPLUS

CN 1,3-Benzenedicarboxamide, N,N'-bis[6-[(2-pyridinylcarbonyl)amino]-2-pyridinyl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 50 THERE ARE 50 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 14 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 2003:950836 HCAPLUS
DOCUMENT NUMBER: 140:16722
TITLE: Preparation of 1,1-disubstituted cycloalkyl derivatives as factor Xa inhibitors for treating a thromboembolic disorder
INVENTOR(S): Qiao, Jennifer X.; Pinto, Donald J.; Orwat, Michael J.; Han, Wei; Friedrich, Sarah R.
PATENT ASSIGNEE(S): Bristol-Myers Squibb Company, USA
SOURCE: PCT Int. Appl., 686 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE

h eb c g cg b cg eb

WO 2003099276 A1 20031204 WO 2003-US13893 20030505
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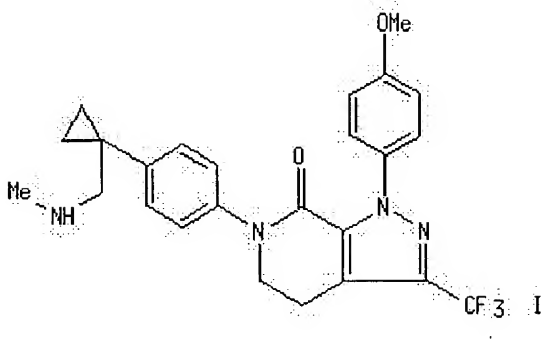
PRIORITY APPLN. INFO.: US 2002-379357P P 20020510
US 2002-415367P P 20021002
OTHER SOURCE(S): MARPAT 140:16722
GI



AB The present application describes 1,1-disubstituted cycloalkyl compds. and derivs. thereof (P4-P-M-M4; variables defined below; most of the examples contain 1,4,5,6-tetrahydro-7H-pyrazolo[3,4-c]pyridin-7-one, e.g. the trifluoroacetate of I), or pharmaceutically acceptable salt forms thereof, which are useful as inhibitors of factor Xa for treatment of a thromboembolic disorder. Although the methods of prepn. are not claimed, ~240 example prepns. are included. A no. of I exhibit Ki's of <10 μM towards factor Xa; also some I are direct acting inhibitors (Ki < 10 μM) of the serine protease thrombin as indicated by their ability to inhibit the cleavage of small mol. substrates by thrombin in a purified system; the specific compds. are not stated. For I: M is a 3-10 membered carbocycle or a 4-10 membered heterocycle, consisting of: C atoms and 1-3 heteroatoms = O, S(O)p, N, and NZ2; ring M is substituted with 0-3 R1a and 0-2 carbonyl groups, and there are 0-3 ring double bonds; P is fused onto ring M and is a 5, 6, or 7 membered carbocycle or a 5, 6, or 7 membered heterocycle, consisting of: C atoms and 1-3 heteroatoms = O, S(O)p, and N; ring P is substituted with 0-3 R1a and 0-2 carbonyl groups, and there are 0-3 ring double bonds; alternatively, ring P is absent and P4 is directly attached to ring M, provided that when ring P is absent, P4 and M4 are attached to the 1,2, 1,3, or 1,4 positions of ring M. One of P4 and M4 is -Z-A-B and the other -G1-G, provided that P4 and M4 are attached to different rings when ring P is present; G is consists of 2 fused rings D and E (ring D, including the two atoms of Ring E to which it is attached, is a 5-6 membered ring consisting of carbon atoms and 0-2 heteroatoms selected from the group consisting of N, O, and S(O)p; E is selected from (un)substituted Ph, pyridyl, pyrimidyl, pyrazinyl, and pyridazinyl; alternatively, ring D is absent and ring E is selected from (un)substituted Ph, pyridyl, pyrimidyl, pyrazinyl, pyridazinyl, pyrrolyl,

h eb c g cg b cg eb

pyrazolyl, imidazolyl, isoxazolyl, oxazolyl, triazolyl, thienyl, and thiazolyl); G1 is absent or = (CR3R3a)1-5, etc. A = (un)substituted C3-10 carbocycle and 5-12 membered heterocycle consisting of: C atoms and 1-4 heteroatoms N, O, and S(O)p; B is Y-R4a or X-Y-R4a, provided that Z and B are attached to different atoms on A and A and R4a or X and R4a are attached to the same atom on Y; Z = a bond, -(CR3R3e)1-4-, etc. Addnl. details including provisos are given in the claims.

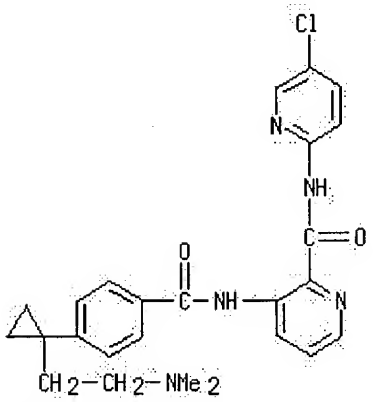
IT **630389-32-1P**

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; prepn. of 1,1-disubstituted cycloalkyl derivs. as factor Xa inhibitors for treating thromboembolic disorder)

RN 630389-32-1 HCAPLUS

CN 2-Pyridinecarboxamide, N-(5-chloro-2-pyridinyl)-3-[[4-[1-[2-(dimethylamino)ethyl]cyclopropyl]benzoyl]amino]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 15 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 2003:945402 HCAPLUS
DOCUMENT NUMBER: 140:769
TITLE: Benzoazepine derivatives as Meniere's disease remedies
INVENTOR(S): Matsukawa, Utane; Fujimori, Akira; Arai, Yukinori; Sudo, Katsumi
PATENT ASSIGNEE(S): Yamanouchi Pharmaceutical Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 20 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2003342175	A2	20031203	JP 2002-149965	20020524
PRIORITY APPLN. INFO.:			JP 2002-149965	20020524

OTHER SOURCE(S): MARPAT 140:769
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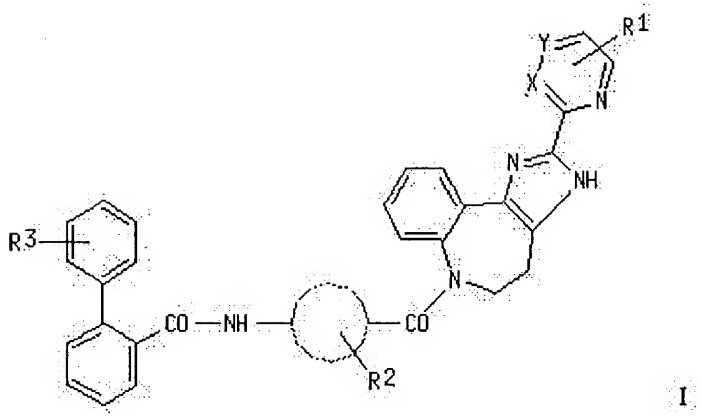


I

AB The new 1,4,5,6-tetrahydroimidazo[4,5-d]benzoazepine derivs. (I; ring D = phenylene, pyridindiyl; X, Y = CH, N; R1, R2, R3 = H, OH, halogen, low alkyl) and their pharmaceutically acceptable salts are claimed as Meniere's disease and hearing disorder remedies. I were prepd., and formulation examples of injections and capsules were given.

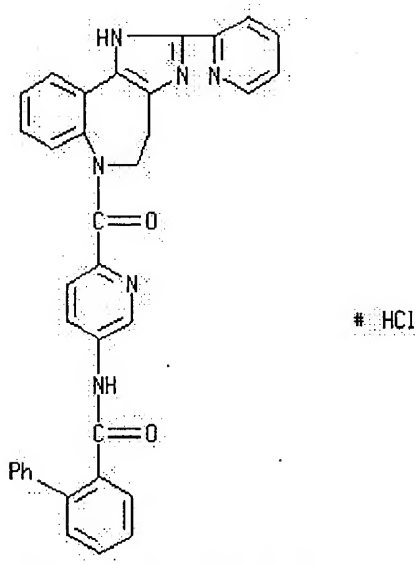
IT **433263-40-2P**

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(benzoazepine derivs. as Meniere's disease remedies)

RN 433263-40-2 HCAPLUS

CN [1,1'-Biphenyl]-2-carboxamide, N-[6-[[4,5-dihydro-2-(2-pyridinyl)imidazo[4,5-d][1]benzazepin-6(1H)-yl]carbonyl]-3-pyridinyl]-, monohydrochloride (9CI) (CA INDEX NAME)



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L12 ANSWER 16 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Cited References

ACCESSION NUMBER: 2003:851478 HCAPLUS

DOCUMENT NUMBER: 140:60070

TITLE: The Effect of Global Compaction on the Local Secondary Structure of Folded Dendrimers

AUTHOR(S): Huang, Baohua; Prantil, Matthew A.; Gustafson, Terry L.; Parquette, Jon R.

h eb c g cg b cg eb

CORPORATE SOURCE: Department of Chemistry, The Ohio State University, Columbus, OH, 43210, USA
SOURCE: Journal of the American Chemical Society (2003), 125(47), 14518-14530
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The effect of nonlocal interactions on the local structural propensities of folded dendrimers was evaluated by comparing, under identical conditions, the conformational properties of isomeric dendrimers differing in their global packing efficiency. A modular synthesis of two series of dendrimers up to the third generation was developed to provide efficient access to isomeric dendrimers displaying different levels of overall compaction. Dendrimer compaction levels were adjusted by connecting the folded dendrons to 1,3,5-benzenetricarbonyl chloride, as the central core, via either a 2- or a 4-aminobenzamide linkage to induce relatively compacted or expanded conformations, resp. The hydrodynamic vol. of the dendrimers was measured by time-resolved fluorescence anisotropy (TRFA) as a function of the dendrimer series, generation level, and solvent. Packing efficiency (compaction level) was estd. by the ratio (Vh/Vvw) of the exptl. hydrodynamic vol. (Vh) to the calcd. van der Waals vol. (Vvw). The extent and stability of local helical bias was measured using CD and correlated with the packing efficiency (Vh/Vvw). Compaction plays an extremely important role in detg. the secondary structural preferences of the dendrimers; however, the nature of compaction was more important than the extent of compaction.

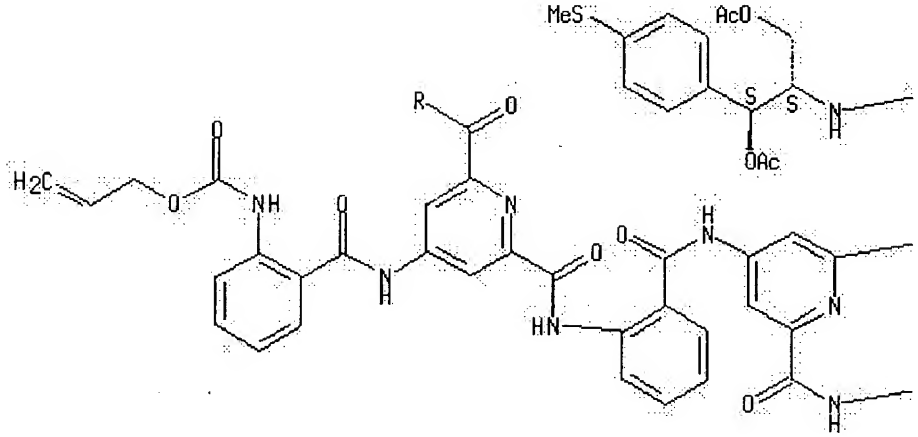
IT **638128-32-2P**
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
([G2]-o-link-N-alloc dendrimer; modular synthesis and effect of global compaction on local secondary structure of folded isomeric dendrimers from CD and fluorescence anisotropy data)

RN 638128-32-2 HCAPLUS

CN Carbamic acid, [2-[[[2,6-bis[[[2-[[[2,6-bis[[[2-[[[(1S,2S)-2-(acetyloxy)-1-[(acetyloxy)methyl]-2-[4-(methylthio)phenyl]ethyl]amino]carbonyl]phenyl]amino]carbonyl]-4-pyridinyl]amino]carbonyl]phenyl]amino]carbonyl]-4-pyridinyl]amino]carbonyl]phenyl]-, 2-propenyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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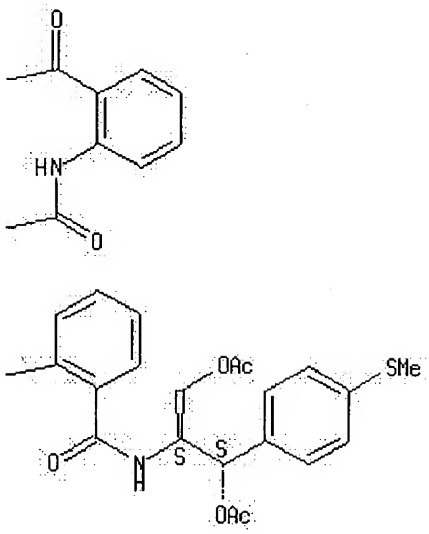
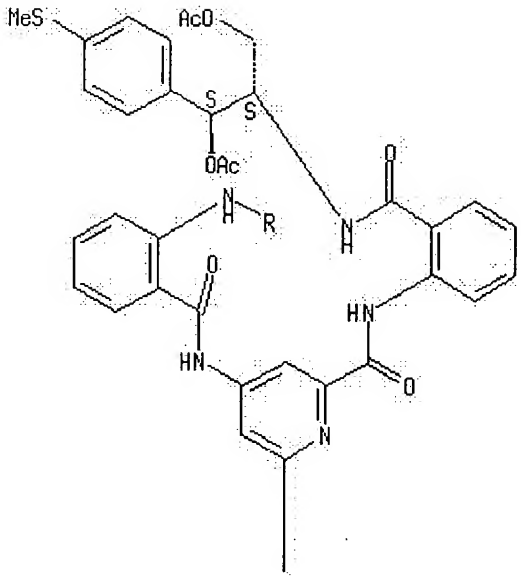
PAGE 1-B



PAGE 2-A



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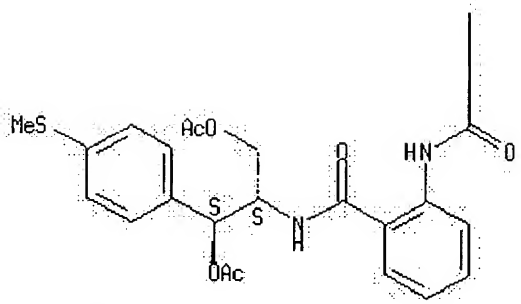

REFERENCE COUNT: 106 THERE ARE 106 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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L12 ANSWER 17 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 2003:528697 HCAPLUS
DOCUMENT NUMBER: 139:223608
TITLE: Effect of Polymer Concentration on Partitioning and Molecular Recognition in Plasticized Poly(vinyl chloride)
AUTHOR(S): Zhang, Xu; Zhao, Hong; Chen, Zhi; Nims, Raymond; Weber, Stephen G.
CORPORATE SOURCE: Department of Chemistry, University of Pittsburgh, Pittsburgh, PA, 15260, USA
SOURCE: Analytical Chemistry (2003), 75(16), 4257-4264
CODEN: ANCHAM; ISSN: 0003-2700
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Mixts. of poly(vinyl chloride) (PVC) with plasticizers have been used in ion-selective electrodes for many years. The same material has proven useful in solid-phase microextn. (SPME), both with and without artificial receptors. The authors hypothesized that by changing the polymer concn. in plasticized PVC membranes contg. artificial receptor from the std. 33 wt. %, the selectivity of the extn. of barbiturates over similar mols. could be improved. Partition coeffs. and receptor-substrate formation consts. of a target species, phenobarbital, in membranes with various polymer concns. were detd. Diffusion coeffs. of the solute phenobarbital in receptor-free membranes were also detd. Kamlet-Taft solvatochromic properties β and π* were measured for the PVC/dioctyl sebacate materials. Cohesive energy densities were calcd. for the same materials. Partition coeffs. for phenobarbital (from aq. soln. to membrane) decrease as [PVC] increases, while the formation consts. for the complex of the solute with its receptor increase. Diffusion coeffs. decrease as the polymer concn. increases as well. The increase in polymer concn. brings about a decrease in hydrogen-bonding basicity and an increase in dipolarity and cohesive energy d. The values of the solvatochromic parameters detd. at various compns. are highly correlated; thus, it is impossible to calc. how much each factor contributes to the changes assocd. with partition and complex formation. The solvatochromic "polarizability correction factor" has been detd. to be 0 for PVC. In SPME expts. at 30%, 40%, and 50% (wt./wt.) PVC, as polymer concn. increases, selectivity for barbiturate extn. over other cyclic imides becomes better in the presence of barbiturate receptor and worse without receptor.

IT **228271-35-0**
RL: ARU (Analytical role, unclassified); ANST (Analytical study)
(effect of polymer concn. on partitioning and mol. recognition in plasticized poly(vinyl chloride) and application to extn. of barbiturates from aq. soln. using artificial receptor)

RN 228271-35-0 HCAPLUS
CN 1,3-Benzenedicarboxamide, N,N'-bis[6-[(2-ethyl-1-oxohexyl)amino]-2-pyridinyl]- (9CI) (CA INDEX NAME)

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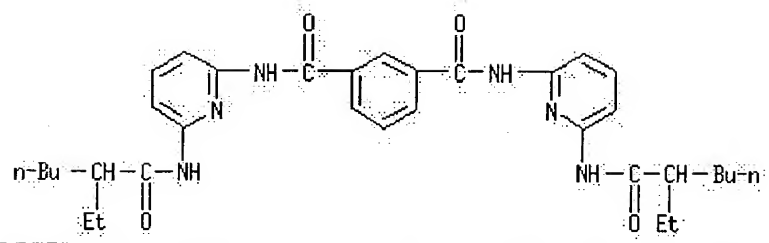

REFERENCE COUNT: 49 THERE ARE 49 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 18 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Refs

ACCESSION NUMBER: 2003:528288 HCAPLUS
DOCUMENT NUMBER: 139:223715
TITLE: Anti-HIV Activity of HEPT, TIBO, and Cyclic Urea Derivatives: Structure-Property Studies, Focused Combinatorial Library Generation, and Hits Selection Using Substructural Molecular Fragments Method
AUTHOR(S): Solov'ev, V. P.; Varnek, A.
CORPORATE SOURCE: Institute of Physiologically Active Compounds, Russian Academy of Sciences, Chernogolovka, 142432, USA
SOURCE: Journal of Chemical Information and Computer Sciences (2003), 43(5), 1703-1719
CODEN: JCISD8; ISSN: 0095-2338
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Substructural mol. fragments (SMF) method [Solov'ev, V. P.; Varnek, A.; Wipff, G. J. Chem. Inf. Comput. Sci. 2000, 40, 847-858] was applied to assess anti-HIV activity for large data sets for three families of compds.: 1-[2-hydroxyethoxymethyl]-6-(phenylthio)thymine (HEPT) derivs., tetrahydroimidazobenzodiazepinone (TIBO) derivs., and cyclic urea (CU) derivs. The SMF method uses 49 types of topol. descriptors (atom/bond sequences and "augmented atoms") which, being coupled with 3 linear and nonlinear fitting equations, allows the user to generate up to 147 structure-property models. For each family of compds., the modeling was performed on several training sets followed by the validation calcns. where three best fit models were applied. Calcd. activities well reproduce available exptl. data. On the basis of the "optimal" mol. fragments, the focused combinatorial library contg. 252 virtual HEPT derivs. has been generated. Its filtering led to several hits potentially possessing anti-HIV activity.

IT **183854-97-9**
RL: BUU (Biological use, unclassified); PAC (Pharmacological activity); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(anti-HIV activity of HEPT, TIBO, and cyclic urea derivs. and structure-property studies, focused combinatorial library generation, and hits selection using substructural mol. fragments method)

RN 183854-97-9 HCAPLUS
CN Benzamide, 3,3'-[[(4R,5S,6S,7R)-tetrahydro-5,6-dihydroxy-2-oxo-4,7-bis(phenylmethyl)-1H-1,3-diazepine-1,3(2H)-diyl]bis(methylene)]bis[N-(6-methyl-2-pyridinyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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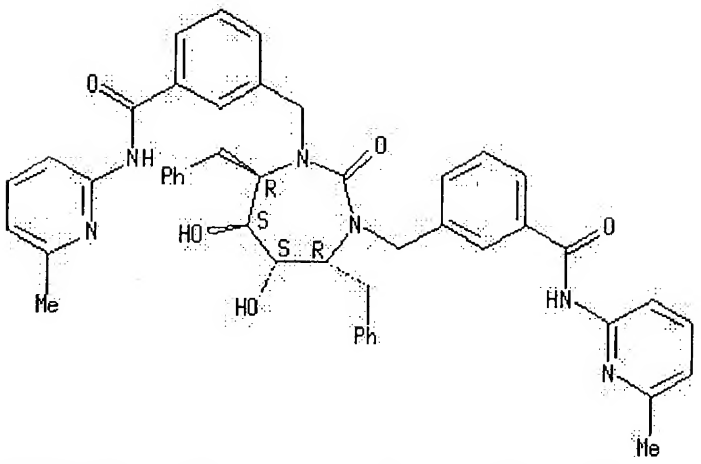

REFERENCE COUNT: 69 THERE ARE 69 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 19 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 2003:472489 HCAPLUS
DOCUMENT NUMBER: 139:53037
TITLE: Preparation of substituted heterocyclic carboxamides with antithrombotic activity
INVENTOR(S): Herron, David Kent; Joseph, Sajan; Marquart, Angela Lynn; Masters, John Joseph; Mendel, David; Smith, Gerald Floyd; Tebbe, Anne Louise; Waid, Philip Parker; Wiley, Michael Robert; Yee, Ying Kwong
PATENT ASSIGNEE(S): Eli Lilly and Company, USA; et al.
SOURCE: PCT Int. Appl., 102 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003050088	A1	20030619	WO 2002-US36139	20021202

W: AE, AG, AL, AM, AT, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, CZ, DE, DE, DK, DK, DM, DZ, EC, EE, EE, ES, FI, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ, BY

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: US 2001-338337P P 20011207
OTHER SOURCE(S): MARPAT 139:53037
GI

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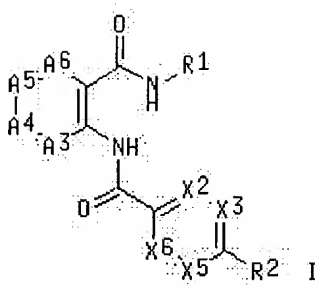

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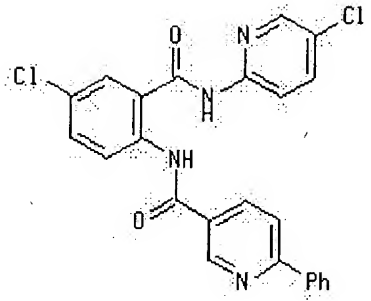


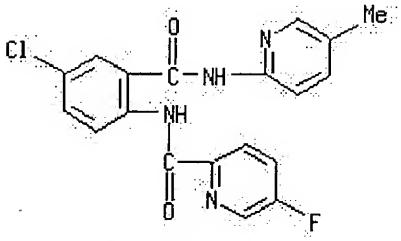
II

AB The title compds. [I; A3-A6, together with the two carbons to which they are attached, complete a substituted benzene or pyridine; R1 = (un)substituted 2-pyridyl; one or two of X1-X4 = N and each of others of X1-X4 = CH; R2 = (un)substituted Ph, 5-6 membered heteroaryl, etc.], useful as inhibitors of factor Xa, were prepd. Thus, coupling 5-chloro-2-(6-chloropyridin-3-ylcarbonylamino)-N-(5-chloropyridin-2-yl)benzamide (prepn. given) with phenylboronic acid afforded the pyridinecarboxamide II. In general, the compds. I exhibit a Kass of 3-10x106 L/Mol or greater against factor Xa (Kass is calcd. for a range of concns. of test compds. which produce hydrolysis inhibition between 20% and 80% of control and the mean value reported in units of liter per mol).

IT **395684-75-0P**, 5-Chloro-2-((5-fluoropyridin-2-ylcarbonyl)amino)-N-(5-methylpyridin-2-yl)benzamide
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of substituted heterocyclic carboxamides with antithrombotic activity)

RN 395684-75-0 HCAPLUS

CN 2-Pyridinecarboxamide, N-[4-chloro-2-[[(5-methyl-2-pyridinyl)amino]carbonyl]phenyl]-5-fluoro- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 20 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 2003:434537 HCAPLUS
DOCUMENT NUMBER: 139:22020
TITLE: Preparation of cyclic amides as apolipoprotein B inhibitors
INVENTOR(S): Takasugi, Hisashi; Inoue, Yoshikazu; Terasawa, Takeshi; Nagayoshi, Akira; Furukawa, Yoshiro; Mikami, Masafumi; Hinoue, Kazumasa; Ohtsubo, Makoto; Fukumoto, Daisuke
PATENT ASSIGNEE(S): Fujisawa Pharmaceutical Co., Ltd., Japan; Daiso Co., Ltd.
SOURCE: PCT Int. Appl., 297 pp.
CODEN: PIXXD2

h eb c g cg b cg eb

DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003045921	A1	20030605	WO 2002-JP11034	20021024
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WO 2002090347	A1	20021114	WO 2002-JP3529	20020409
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PRIORITY APPLN. INFO.:		
AU 2001-9164	A	20011128
AU 2002-443	A	20020211
TW 2002-91106855	A	20020404
WO 2002-JP3529	A	20020409
AU 2001-4722	A	20010430
AU 2002-9937	A	20020111

OTHER SOURCE(S): MARPAT 139:22020

AB The present invention relates to R1XC(O)NH-A-Z-Y-R2 (1; mostly 2-phenyl-1-cycloalkenecarboxamides and 1,1'-biphenyl-2-carboxamides) wherein R1 is (un)substituted aryl; R2 is (un)substituted aryl, (un)substituted heteroaryl, (un)substituted lower cycloalkyl, (un)substituted aryloxy, (un)substituted arylsulfonyl, vinyl, carbamoyl, protected carboxy or protected amino; ring A is bivalent residue derived from (un)substituted aryl or (un)substituted heteroaryl; X is bivalent residue derived from cycloalkene, naphthalene, unsatd. 5 or 6-membered heteromonocyclic group, each of which is (un)substituted, and substituted benzene; Y is -(A1)m1-(A2)m2- (A1 is -NH-, -N(R3)-, -CO-, -NHCO-, -CONH-, -COCH:CH-, -O-, -CH2O-, -CH2NHCO-, -CH2CONH or -CH(OH)-, wherein R3 is amino protective group, A2 is lower alkylene (un)substituted by aryl, and m1 and m2 = 0 or 1); and Z is direct bond or piperazine, or a salt thereof. Compds. 1 (e.g. 4'-chloro-4-methyl-N-[4-[[2-(2-pyridinyl)ethyl]amino]phenyl]-1,1'-biphenyl-2-carboxamide) inhibit apolipoprotein B (Apo B) secretion and are useful as a medicament for prophylactic and treatment of diseases or conditions resulting from elevated circulating levels of Apo B. For example, 4'-chloro-4-methyl-N-[4-[[2-(2-pyridinyl)ethyl]amino]phenyl]-1,1'-biphenyl-2-carboxamide exhibited 95% inhibition of Apo B secretion at 10-8 M; also, it lowered cholesterol and triglyceride levels in ddY-mice by 86 and 36%, resp. after 2 h. Example prepns. of >400 1 and 187 intermediates are included. For example, 2-isopropyl-N-[4-[[2-(2-pyridinyl)ethyl]amino]phenyl]-4-[4-(trifluoromethyl)phenyl]-5-pyrimidinecarboxamide (366 mg) was prepd. from

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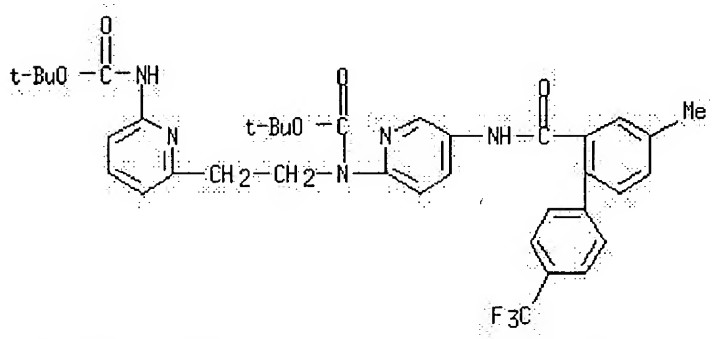
2-isopropyl-4-[4-(trifluoromethyl)phenyl]-5-pyrimidinecarboxylic acid (495 mg), tert-Bu 4-aminophenyl[2-(2-pyridinyl)ethyl]carbamate (470 mg) and 1-hydroxybenzotriazole hydrate (223 mg) and 1-[3-(dimethylamino)propyl]-3-ethylcarbodiimide hydrochloride (315 mg) in N,N-dimethylformamide (20 mL) followed by CF3CO2H. The reactant tert-Bu 4-aminophenyl[2-(2-pyridinyl)ethyl]carbamate (15.03 g) was prepd. from tert-Bu 4-nitrophenyl[2-(2-pyridinyl)ethyl]carbamate (20.03 g) in ethanol (400 mL) and iron(III) chloride (189 mg) and active charcoal (20 g) followed by hydrazine hydrate (11.67 g).

IT **537716-57-7P**, tert-Butyl [2-[6-[(tert-butoxycarbonyl)amino]-2-pyridinyl]ethyl][5-[[[4-methyl-4'-(trifluoromethyl)-1,1'-biphenyl-2-yl]carbonyl]amino]-2-pyridinyl]carbamate
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(drug candidate; prepn. of cyclic amide compds. as apolipoprotein B secretion inhibitors)

RN 537716-57-7 HCAPLUS

CN Carbamic acid, [2-[6-[[(1,1-dimethylethoxy)carbonyl]amino]-2-pyridinyl]ethyl][5-[[[4-methyl-4'-(trifluoromethyl)[1,1'-biphenyl]-2-yl]carbonyl]amino]-2-pyridinyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 21 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 2003:242097 HCAPLUS
DOCUMENT NUMBER: 138:267201
TITLE: Pesticidal compositions for coating plant propagation material containing anthranilamides
INVENTOR(S): Berger, Richard Alan; Flexner, John Lindsey
PATENT ASSIGNEE(S): E. I. Du Pont de Nemours & Co., USA
SOURCE: PCT Int. Appl., 147 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003024222	A1	20030327	WO 2002-US30302	20020910

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,

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LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

EP 1427285 A1 20040616 EP 2002-775972 20020910

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK

PRIORITY APPLN. INFO.: US 2001-323941P P 20010921

WO 2002-US30302 W 20020910

OTHER SOURCE(S): MARPAT 138:267201

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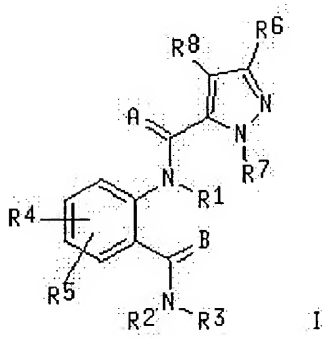


I

AB An invertebrate pest control compn. for coating a propagule comprises (1) a biol. effective amt. of an anthranilamide compds. I (Markush included), an N-oxide thereof or an agriculturally suitable salt thereof, and (2) a film former or adhesive agent. Arthropodicidal compn. contg. anthranilamide compds. I may further comprise addnl. biol. active compds. selected from arthropodicides of the group consisting of pyrethroids, carbamates, neonicotinoids, neuronal sodium channel blockers, insecticidal macrocyclic lactones, γ-aminobutyric acid (GABA) antagonists, insecticidal ureas, and juvenile hormone mimics, and fungicides. The propagule is a seed of cotton, maize, soybean, rice, etc., or a rhizome, tuber, bulb or corm, or viable division thereof, of potato, sweet potato, garden onion, tulip, daffodil, crocus hyacinth, etc., or is a stem or leaf cutting.

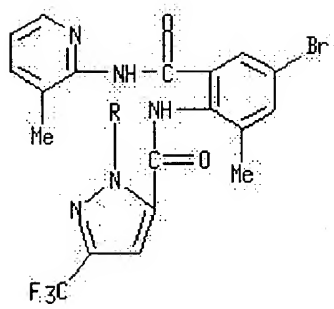
IT **500009-40-5**

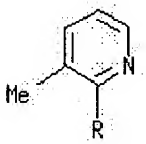
RL: AGR (Agricultural use); BSU (Biological study, unclassified); BIOL (Biological study); USES (Uses)

(anthranilamide compds. as pesticides for plant propagation material)

RN 500009-40-5 HCAPLUS

CN 1H-Pyrazole-5-carboxamide, N-[4-bromo-2-methyl-6-[[(3-methyl-2-pyridinyl)amino]carbonyl]phenyl]-1-(3-methyl-2-pyridinyl)-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)





REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 22 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 2003:199730 HCAPLUS
DOCUMENT NUMBER: 138:337665
TITLE: Weak C-H/π Interaction Participates in the Diastereoselectivity of a Host-Guest Complex in the Presence of Six Strong Hydrogen Bonds
AUTHOR(S): Frontera, Antonio; Garau, Carolina; Quinonero, David; Ballester, Pablo; Costa, Antoni; Deya, Pere M.
CORPORATE SOURCE: Departament de Quimica, Universitat de les Illes Balears, Palma de Mallorca, 07122, Spain
SOURCE: Organic Letters (2003), 5(7), 1135-1138
CODEN: ORLEF7; ISSN: 1523-7060
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

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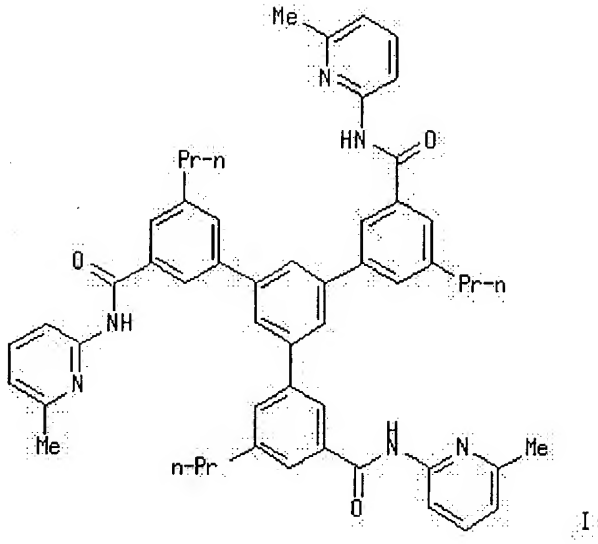


I

AB We report a study of the interaction between methylmethanetriacetic acid (MMTA) and a tripodal amidopyridine receptor 1 (I), where the geometry of the binding is in part governed by a weak C-H/π interaction in the presence of six strong N(O)-H···O(N) hydrogen bonds. There are two possible binding geometries for the 1:1 complex 1·MMTA; combining computational and exptl. evidence we demonstrate that the endo binding mode is more favorable as the result of a C-H/π interaction.

IT **484052-54-2**

RL: PRP (Properties)

(H-bonding interactions and in-out stereoisomerism; weak C-H/π interaction participates in the diastereoselectivity of a host-guest complex in the presence of six strong hydrogen bonds)

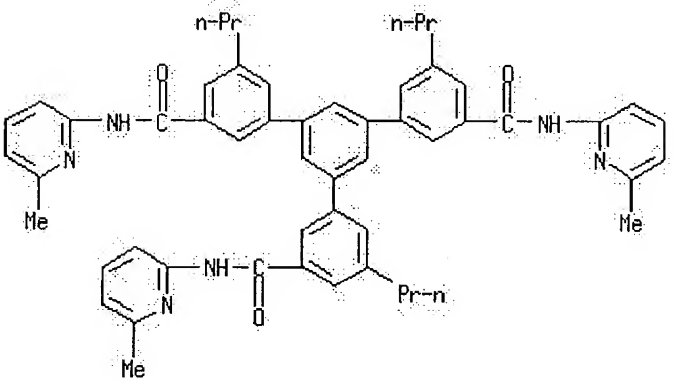
RN 484052-54-2 HCAPLUS

CN Pentanedioic acid, 3-(carboxymethyl)-3-methyl-, compd. with N,N'-bis(6-methyl-2-pyridinyl)-5'-[3-[[(6-methyl-2-pyridinyl)amino]carbonyl]-5-propylphenyl]-5,5''-dipropyl[1,1':3',1''-terphenyl]-3,3''-dicarboxamide (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 221021-04-1

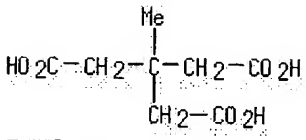
CMF C54 H54 N6 O3



CM 2

h eb c g cg b cg eb

CRN 85963-71-9
CMF C8 H12 O6



REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 23 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 2003:154243 HCAPLUS
DOCUMENT NUMBER: 138:204839
TITLE: Preparation of benzamides affecting glucokinase for combined treatment or prevention of type 2 diabetes and obesity
INVENTOR(S): Boyd, Scott; Caulkett, Peter William Rodney; Hargreaves, Rodney Brian; Bowker, Suzanne Saxon; James, Roger; Johnstone, Craig; Jones, Clifford David; McKerrecher, Darren; Block, Michael Howard
PATENT ASSIGNEE(S): Astrazeneca AB, Swed.; Astrazeneca UK Limited
SOURCE: PCT Int. Appl., 156 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003015774	A1	20030227	WO 2002-GB3745	20020815
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
EP 1420784	A1	20040526	EP 2002-755165	20020815
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK				

PRIORITY APPLN. INFO.: SE 2001-2764 A 20010817
WO 2002-GB3745 W 20020815

OTHER SOURCE(S): MARPAT 138:204839
GI

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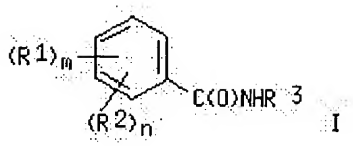
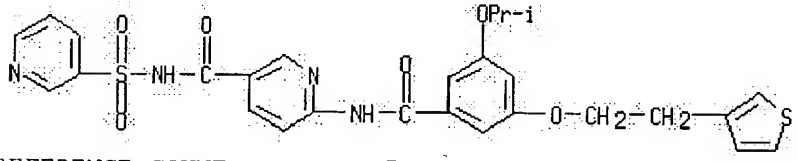


AB The invention relates to the use of benzamides (shown as I; variables defined below; e.g. 2-[[3,5-di(2-chlorobenzyloxy)benzoyl]amino]thiazole) or a salt, solvate or prodrug thereof, in the prepn. of a medicament for the treatment or prevention of a disease condition mediated through glucokinase (GLK; no data), such as type 2 diabetes, and to the compds. I and methods for prepg. them. Twelve pharmaceutical compns. are included. For I: m is 0-2; n is 0-4; and n + m > 0; each R1 = OH, -(CH2)1-4OH, -CH3-aFa, -(CH2)1-44CH3-aFa, -OCH3-aFa, halo, C1-6alkyl, C2-6alkenyl, C2-6alkynyl, NH2, -NH-C1-4alkyl, -N-di(C1-4alkyl), CN, formyl, Ph or heterocyclyl optionally substituted by C1-6alkyl. Each R2 is the group Y-X- wherein each X is a linker = -O-Z-, -O-Z-O-Z-, -C(O)O-Z-, -OC(O)-Z-, -S-Z-, -SO-Z-, -SO2-Z-, -N(R6)-Z-, -N(R6)SO2-Z-, -SO2N(R6)-Z-, -(CH2)1-4-, -CH:CH-Z-, -C≡C-Z-, -N(R6)CO-Z-, -CON(R6)-Z-, -C(O)N(R6)S(O)2-Z-, -S(O)2N(R6)C(O)-Z-, -C(O)-Z-, -Z-, -C(O)-Z-O-Z-, -N(R6)-C(O)-Z-O-Z-, -O-Z-N(R6)-Z-, -O-C(O)-Z-O-Z- or a direct bond; each Z = a direct bond, C2-6alkenylene or -(CH2)p-C(R6a)2-(CH2)q-; each Y = aryl-Z1-, heterocyclyl-Z1-, C3-7cycloalkyl-Z1-, C1-6alkyl, C2-6alkenyl, C2-6alkynyl, -(CH2)1-4CH3-aFa or -CH(OH)CH3-aFa; R3 = Ph or a heterocyclyl; addnl. details are given in the claims. More than 30 example prepns. of I are included and >300 specific examples of I are included with characterization data. For example, to prep. 2-[[3,5-di(2-chlorobenzyloxy)benzoyl]amino]thiazole, diisopropylethylamine (2.0 mmol) then 4-dimethylaminopyridine (0.1 mmol) were added to a soln. of 2-aminothiazole (1.0 mmol) and 3,5-di(2-chlorobenzyloxy)benzoic acid chloride (1.0 mmol) in CH2Cl2 (10 mL) under Ar at ambient temp. After 80 mins the reaction mixt. was filtered, washed with CH2Cl2 and dried under high vacuum to give the title compd. as a colorless solid (41%).

IT **499991-30-9P**, N-(5-((((Pyridin-3-yl)sulfonyl)amino)carbonyl)pyridin-2-yl)-3-isopropoxy-5-(2-(thien-3-yl)ethoxy)benzamide
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; prepn. of benzamides affecting glucokinase for combined treatment or prevention of type 2 diabetes and obesity)

RN 499991-30-9 HCAPLUS

CN 3-Pyridinecarboxamide, 6-[[3-(1-methylethoxy)-5-[2-(3-thienyl)ethoxy]benzoyl]amino]-N-(3-pyridinylsulfonyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 24 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 2003:154154 HCAPLUS
DOCUMENT NUMBER: 138:200331

h eb c g cg b cg eb

TITLE: Method for controlling particular insect pests by applying anthranilamide compounds

INVENTOR(S): Lahm, George Philip; McCann, Stephen Frederick; Patel, Kanu Maganbhai; Selby, Thomas Paul; Stevenson, Thomas Martin

PATENT ASSIGNEE(S): E. I. Du Pont de Nemours & Co., USA

SOURCE: PCT Int. Appl., 150 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 4

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003015518	A1	20030227	WO 2002-US25613	20020813
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
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EP 1416796	A1	20040512	EP 2002-752809	20020813
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK				

PRIORITY APPLN. INFO.:

US 2001-311919P	P	20010813
US 2001-324173P	P	20010921
WO 2002-US25613	W	20020813

OTHER SOURCE(S): MARPAT 138:200331

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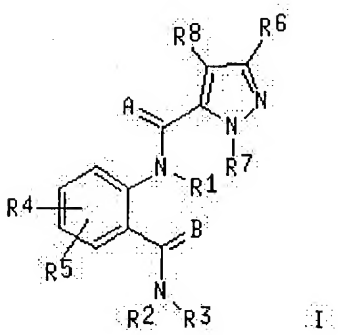

I

AB Anthranilamide compds. I (Markush included), N-oxides or an agriculturally suitable salts thereof are prepd. as insecticides for controlling lepidopteran, homopteran, hemipteran, thysanopteran and coleopteran insect pests. Insecticidal compn. contg. anthranilamide compds. I may further comprise addnl. biol. active compds. selected from arthropodicides of the group consisting of pyrethroids, carbamates, neonicotinoids, neuronal sodium channel blockers, insecticidal macrocyclic lactones, γ-aminobutyric acid (GABA) antagonists, insecticidal ureas, and juvenile hormone mimics.

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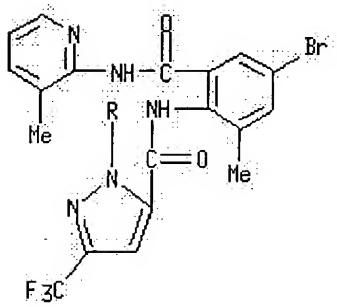
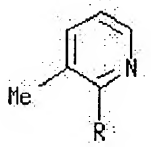
IT 500009-40-5
RL: AGR (Agricultural use); BSU (Biological study, unclassified); BIOL (Biological study); USES (Uses)
(anthranilamide compds. as insecticides)
RN 500009-40-5 HCAPLUS
CN 1H-Pyrazole-5-carboxamide, N-[4-bromo-2-methyl-6-[[(3-methyl-2-pyridinyl)amino]carbonyl]phenyl]-1-(3-methyl-2-pyridinyl)-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)





REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 25 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | More References

ACCESSION NUMBER: 2003:5785 HCAPLUS
DOCUMENT NUMBER: 138:73180
TITLE: Preparation of amino-nicotinate derivatives for therapeutic use as glucokinase (GLK) modulators
INVENTOR(S): Hayter, Barry Raymond; Currie, Gordon Stuart; Hargreaves, Rodney Brian; James, Roger; Jones, Clifford David; Mckerrecher, Darren; Allen, Joanne Victoria; Caulkett, Peter William Rodney; Johnstone, Craig; Gaskin, Harold
PATENT ASSIGNEE(S): Astrazeneca AB, Swed.; Astrazeneca UK Limited
SOURCE: PCT Int. Appl., 110 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003000267	A1	20030103	WO 2002-GB2873	20020624

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU,

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TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

EP 1404335	A1	20040407	EP 2002-740900	20020624
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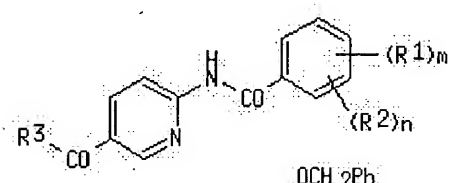
BR 2002010711	A	20040720	BR 2002-10711	20020624
PRIORITY APPLN. INFO.:			SE 2001-2300	A 20010626
			WO 2002-GB2873	W 20020624

OTHER SOURCE(S): MARPAT 138:73180
GI



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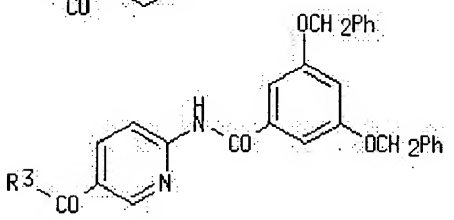
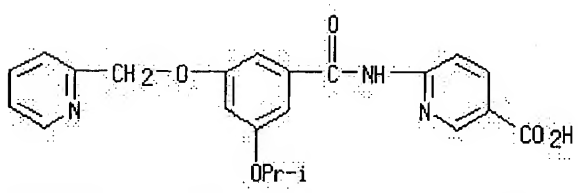


II

AB Aminonicotinates, such as I [R1 = H, OH, (CH2)1-4OH, NO2, NH2, haloalkyl, haloalkyloxy, alkyl, alkenyl, alkylamino, etc.; R2 = X-Y; X = linking group, such as O, CO, amino, Z-O-Z, etc; Z = alkylene, alkenylene, etc.; R3 = OH, alkoxy, alkylamino, etc.; m = 0-2; n = 0-4; m + n > 0], were prepd. for pharmaceutical use in the treatment of diseases or conditions mediated through glucokinase (GLK), such as type 2 diabetes. Thus, nicotinic acid deriv. II (R3 = OH) was prepd. by treatment of 3,5-dibenzyloxybenzoic acid with oxalyl chloride in CH2Cl2 and DMF followed by addn. of Me 6-aminonicotinate to the reaction mixt. form ester II (R3 = OMe) in 57% yield and subsequent hydrolysis of the ester using LiOH in THF/H2O to give the desired acid in 17% yield. The prepd. compds. were assayed for their effect on GLK activity, and pharmaceutical compns. of the prepd. compds. were presented.

IT **480463-03-4P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of amino nicotinate derivs. for therapeutic use as glucokinase (GLK) modulators)

RN 480463-03-4 HCAPLUS
CN 3-Pyridinecarboxylic acid, 6-[[3-(1-methylethoxy)-5-(2-pyridinylmethoxy)benzoyl]amino]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

h eb c g cg b cg eb

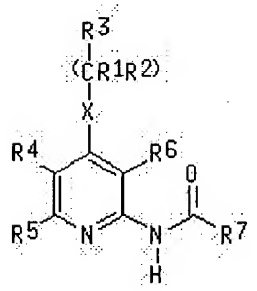
L12 ANSWER 26 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Refs

ACCESSION NUMBER: 2002:927405 HCAPLUS
DOCUMENT NUMBER: 138:14017
TITLE: Preparation of aminoquinoline and aminopyridine derivatives and their use as adenosine a3 ligands
INVENTOR(S): Aranyi, Peter; Balazs, Laszlo; Balogh, Maria; Bata, Imre; Batori, Sandor; Nagy, Lajos T.; Timari, Geza; Boer, Kinga; Finance, Olivier; Kapui, Zoltan; Mikus, Endre; Szamosvoelgyi, Zsuzsanna; Szeleczky, Gabor; Urban-szabo, Katalin
PATENT ASSIGNEE(S): Sanofi-Synthelabo, Fr.
SOURCE: PCT Int. Appl., 51 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002096879	A1	20021205	WO 2002-HU48	20020529
WO 2002096879	C2	20031120		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
EE 200300574	A	20040216	EE 2003-574	20020529
EP 1390349	A1	20040225	EP 2002-732985	20020529
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
BR 2002009719	A	20040727	BR 2002-9719	20020529
PRIORITY APPLN. INFO.:			HU 2001-2279	A 20010531
			HU 2002-774	A 20020301
			WO 2002-HU48	W 20020529

OTHER SOURCE(S): MARPAT 138:14017
GI



I

h eb c g cg b cg eb

AB Aminoquinoline and aminopyridine derivs. [I; wherein R1, R2, independently = H, (branched) (C1-C4)alkyl; R3 = H, (branched) (C1-C4)alkyl, Ph, thienyl, furyl, etc.; R4, R5, independently = H or form together a 1,3-butadienyl group, optionally substituted by methylenedioxy or one or more (branched) (C1-4)alkyl, (C1-C4)alkoxy, hydroxy, halogens; R6 = H, CN, aminocarbonyl, (C1-C4)alkoxycarbonyl, carboxy; R7 = H, (branched) (C1-C4)alkyl, Ph, benzyl, thienyl, furyl, etc.; X = CH2, N, alkylamino, S, O, etc.] were prepd. For example, 3-methyl-N-(4-benzylamino-3-cyanoquinolin-2-yl)benzamide was prepd. by a multistep synthetic procedure. The prepd. compds. are strong adenosine A3 receptor ligands (Ki values in human adenosine A3 receptor binding studies are between 0.19 and 0.69 nM).

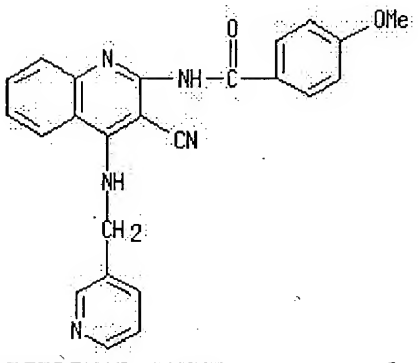
IT **477707-39-4P**

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of aminoquinoline and aminopyridine derivs. and their use as adenosine a3 ligands)

RN 477707-39-4 HCAPLUS

CN Benzamide, N-[3-cyano-4-[(3-pyridinylmethyl)amino]-2-quinolinyl]-4-methoxy- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 27 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 2002:870405 HCAPLUS
DOCUMENT NUMBER: 138:89381
TITLE: Dual Binding Mode of Methylmethanetriacetic Acid to Tripodal Amidopyridine Receptors
AUTHOR(S): Ballester, Pablo; Capo, Magdalena; Costa, Antoni; Deya, Pere M.; Gomila, Rosa; Decken, Andreas; Deslongchamps, Ghislain
CORPORATE SOURCE: Departament de Quimica, Universitat de les Illes Balears, Palma de Mallorca, 07071, Spain
SOURCE: Journal of Organic Chemistry (2002), 67(25), 8832-8841 CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:89381

AB A series of tripodal amidopyridine receptors capable of selective recognition of methylmethanetriacetic acid (MMTA) in org. solvents is described. Intramol. hydrogen-bonding groups, built into some of the receptors, were designed as preorganization devices. Binding was studied

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by NMR titrn., variable temp. NMR expts., 2D-NMR, isothermal titrn. calorimetry, and single-crystal X-ray crystallog. The results reveal that a balancing act between inter- and intramol. hydrogen-bonding interactions in the complexes governs both the dynamics and the geometry of binding. Receptor 1b (without intramol. hydrogen-bonding groups) features a simple sym. MMTA binding geometry with optimal enthalpic interactions. In sharp contrast, receptor 1a (with intramol. hydrogen-bonding groups) reveals a temp.-dependent dual binding mode where MMTA can bind in two completely different geometries. The two soln. binding geometries of 1a·MMTA were unraveled by NMR expts. and correlated to the X-ray structures.

IT **484052-53-1**

RL: FMU (Formation, unclassified); PRP (Properties); FORM (Formation, nonpreparative)

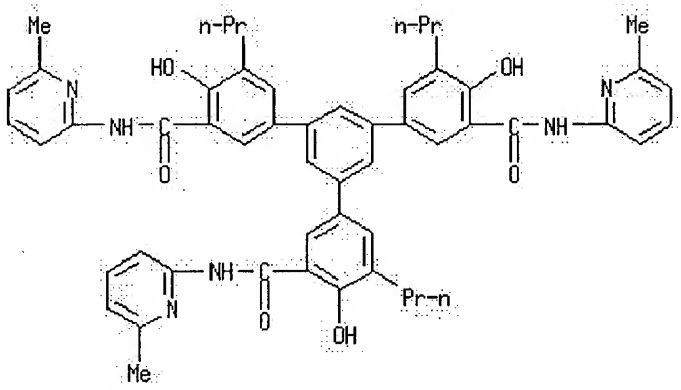
(crystal structure and mol. structure; dual binding mode of methylmethanetriacetic acid to tripodal amidopyridine receptors)

RN 484052-53-1 HCAPLUS

CN Pentanedioic acid, 3-(carboxymethyl)-3-methyl-, compd. with 4,4''-dihydroxy-5'-[4-hydroxy-3-[[(6-methyl-2-pyridinyl)amino]carbonyl]-5-propylphenyl]-N,N'-bis(6-methyl-2-pyridinyl)-5,5''-dipropyl[1,1':3',1''-terphenyl]-3,3''-dicarboxamide (1:1) (9CI) (CA INDEX NAME)

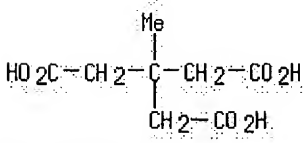
CM 1

CRN 157460-60-1
CMF C54 H54 N6 O6



CM 2

CRN 85963-71-9
CMF C8 H12 O6



REFERENCE COUNT: 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 28 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 2002:868928 HCAPLUS
DOCUMENT NUMBER: 137:352900

h eb c g cg b cg eb

TITLE: Selective anthranilamide pyridine amides as inhibitors of VEGFR-2 and VEGFR-3

INVENTOR(S): Ernst, Alexander; Huth, Andreas; Krueger, Martin; Thierauch, Karl-Heinz; Menrad, Andreas; Haberey, Martin

PATENT ASSIGNEE(S): Schering Aktiengesellschaft, Germany

SOURCE: PCT Int. Appl., 115 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

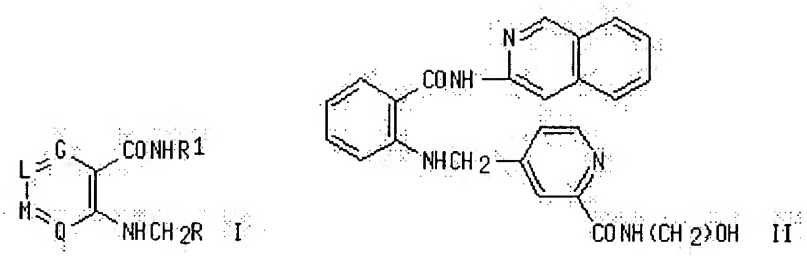
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002090352	A2	20021114	WO 2002-EP4924	20020503
WO 2002090352	A3	20030501		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
DE 10123574	A1	20021128	DE 2001-10123574	20010508
DE 10125294	A1	20021121	DE 2001-10125294	20010515
DE 10164590	A1	20030710	DE 2001-10164590	20011221
EP 1392680	A2	20040303	EP 2002-735333	20020503
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
BR 2002009485	A	20040706	BR 2002-9485	20020503

PRIORITY APPLN. INFO.:

DE 2001-10123574	A	20010508
DE 2001-10125294	A	20010515
DE 2001-10164590	A	20011221
WO 2002-EP4924	W	20020503

OTHER SOURCE(S): MARPAT 137:352900

GI



AB Title compds. I [G, L, M, Q = N, (un)substituted CH, ≤1 of them being N; R = (un)substituted N heterocycle; R1 = (un)substituted alkyl, alkenyl, cycloalkyl, cycloalkenyl, aryl, heteroaryl] were prepd. I are inhibitors of VEGFR-2 and VEGFR-3 and are used as medicaments for treating diseases that are caused by persistent angiogenesis, such as psoriasis, Kaposi's sarcoma, restenosis, such as e.g. stent-induced restenosis, endometriosis, Crohn's disease, Hodgkin's disease, leukemia, arthritis,

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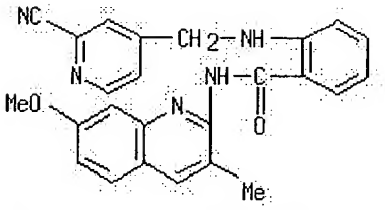
such as rheumatoid arthritis, hemangioma, angiofibromatosis, in eye diseases such as diabetic retinopathy, neovascular glaucoma, in kidney diseases such as glomerulonephritis, diabetic nephropathy, malign nephrosclerosis, thrombic micro-angiopathic syndrome, transplant rejection and glomerulopathy, in fibrotic diseases such as hepatic cirrhosis, mesangial-cell proliferative diseases, arteriosclerosis, damage to the nerve tissue and inhibition of the re-occlusion of vessels after balloon catheter treatment, in vessel prosthetics or after the use of mech. devices for keeping vessels open, e.g. stents, as immunosuppressants, to support wound healing without scars and in cases of age spots and contact dermatitis. I can also be used as inhibitors of VEGFR-3 in lymphangiogenesis for hyperplastic and dysplastic changes in the lymphatic system. Thus, 2-amino-N-isoquinolin-3-ylbenzamide was treated with 2-bromo-5-pyridinecarboxaldehyde, followed by carboxylaton and amidation to give the amide II. II had IC50 for inhibition of VEGFR-2 of 40 nM and for inhibition of cytochrome 450 isoenzyme 2C9 of 2.9 μM.

IT **474799-55-8P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of isoquinolinylcarbamoylphenylaminomethylpyridinecarboxamides as VEGFR-2 and VEGFR-3 inhibitors)

RN 474799-55-8 HCAPLUS

CN Benzamide, 2-[[(2-cyano-4-pyridinyl)methyl]amino]-N-(7-methoxy-3-methyl-2-quinolinyl)- (9CI) (CA INDEX NAME)



L12 ANSWER 29 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | More References

ACCESSION NUMBER: 2002:846211 HCAPLUS
DOCUMENT NUMBER: 138:378554
TITLE: Six-membered cyclic ureas as HIV-1 protease inhibitors: A QSAR study based on CODESSA PRO approach
AUTHOR(S): Katritzky, Alan R.; Oliferenko, Alexander; Lomaka, Andre; Karelson, Mati
CORPORATE SOURCE: Department of Chemistry, Center for Heterocyclic Compounds, University of Florida, Gainesville, FL, 32611-7200, USA
SOURCE: Bioorganic & Medicinal Chemistry Letters (2002), 12(23), 3453-3457
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Quant. structure-activity relationships (QSAR) for HIV-1 protease inhibitory activity of substituted tetrahydropyrimidinones have been produced using CODESSA PRO methodol. and software. The best four-parameter equation (R2cv = 0.847) allowed us to reveal two main structural factors which are strongly correlated with the title activity: mol. hydrophobicity and ability to form hydrogen bonds with the target enzyme.

IT **219941-25-0**

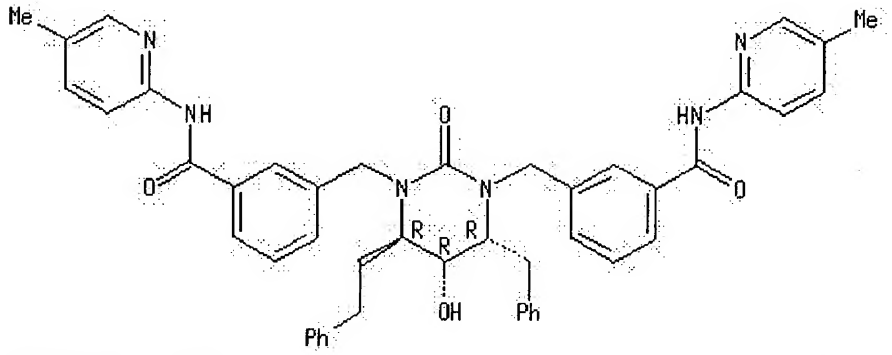
h eb c g cg b cg eb

RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(QSAR study of cyclic ureas as HIV-1 protease inhibitors)

RN 219941-25-0 HCAPLUS

CN Benzamide, 3,3'-[[(4R,5R,6R)-dihydro-5-hydroxy-2-oxo-4-(2-phenylethyl)-6-(phenylmethyl)-1,3(2H,4H)-pyrimidinediyl]bis(methylene)]bis[N-(5-methyl-2-pyridinyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 30 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | More References

ACCESSION NUMBER: 2002:841257 HCAPLUS
DOCUMENT NUMBER: 138:4333
TITLE: Recognition of heteroaromatic molecular tweezers involving multiple hydrogen-bonding sites for neutral molecules
AUTHOR(S): Mu, Qi-Ming; Zhao, Zhi-Ming; Chen, Shu-Hua
CORPORATE SOURCE: Faculty of Chemistry, Sichuan University, Chengdu, 610064, Peop. Rep. China
SOURCE: Huaxue Xuebao (2002), 60(10), 1841-1845
CODEN: HHHPA4; ISSN: 0567-7351
PUBLISHER: Kexue Chubanshe
DOCUMENT TYPE: Journal
LANGUAGE: Chinese

AB Six mol. tweezers have been synthesized based on the incorporation of multiple hydrogen-bonding groups into the cleft to provide both orientation and selective complexation of substrate. Mol. recognition properties of these receptors for barbiturate, urea, diphenylmethanone and glutarimide have been investigated by UV-visible spectroscopic titrn., which indicates that the supramol. complexes consist of 1:1 host and guest mols. The main driving forces are the multiple hydrogen bonding in mol. recognition. The mol. recognition ability is discussed from the viewpoint of the size/shape-fit and geometrical complementary relationship. Computer-aided study and 1H NMR spectroscopy have been employed to elucidate the binding behavior of these mol. tweezers.

IT **476688-57-0**

RL: FMU (Formation, unclassified); FORM (Formation, nonpreparative)
(recognition of heteroarom. mol. tweezers involving multiple hydrogen-bonding sites for neutral mols.)

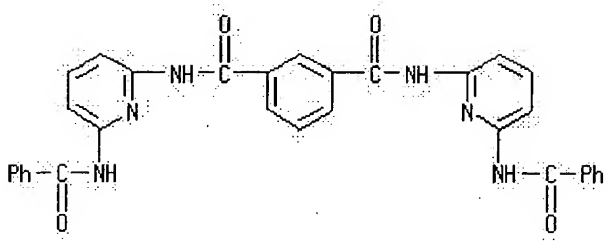
RN 476688-57-0 HCAPLUS

CN 1,3-Benzenedicarboxamide, N,N'-bis[6-(benzoylamino)-2-pyridinyl]-, compd. with urea (1:1) (9CI) (CA INDEX NAME)

h eb c g cg b cg eb

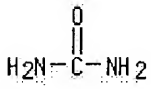
CM 1

CRN 425377-08-8
CMF C32 H24 N6 O4



CM 2

CRN 57-13-6
CMF C H4 N2 O



L12 ANSWER 31 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Many References

ACCESSION NUMBER: 2002:826868 HCAPLUS
DOCUMENT NUMBER: 138:39343
TITLE: Synthesis and Investigation of New Macrocyclic Diphosphine-Palladium(0) Complexes Based on the Barbiturate Binding Receptor
AUTHOR(S): Sorensen, Hanne S.; Larsen, Jens; Rasmussen, Brian S.; Laursen, Bolette; Hansen, Signe G.; Skrydstrup, Troels; Amatore, Christian; Jutand, Anny
CORPORATE SOURCE: Department of Chemistry, University of Aarhus, Aarhus, 8000, Den.
SOURCE: Organometallics (2002), 21(24), 5243-5253
CODEN: ORGND7; ISSN: 0276-7333
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:39343

AB A series of diphosphine ligands possessing a barbiturate-binding receptor, isophthaloylbis(2,6-diaminopyridine) were synthesized with the goal of prepg. new palladium(0) complexes for the auxiliary directed regioselective Heck arylation, which position the alkene with respect to the metal center and thereby control the regioselectivity of the insertion step. Some of the diphosphines prepd. were found to efficiently form macrocyclic bisphosphine palladium(0) complexes even though a 26-membered cycle is produced. A significant solvent effect for the oxidative addn. of the Pd0 complexes with Ph iodide was noted in the case of one of the diphosphine ligands, which was accounted for the ability of the ligand complexed to Pd0 to possess different conformations in the tested solvents, which affects on the diphosphine bite angle. The receptors possessing an isophthaloyl connector bind barbital with affinities corresponding to those of the previously reported open receptors. However, upon complexation with Pd(dba)2, none of the bidentate ligands revealed a capacity to bind barbital, reflecting again the conformational

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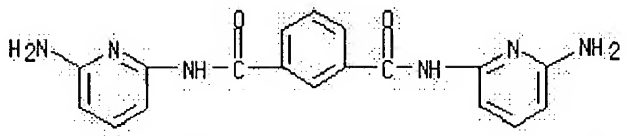
changes that occur upon coordination to Pd0. The new palladium(0) complexes were tested for their ability to promote the Heck reaction between aryl iodides, bromides and chloride and Bu acrylate, providing catalytic activity comparable or better than that of the PPh3 ligand.

IT **112817-57-9**

RL: RCT (Reactant); RACT (Reactant or reagent)
(acylation; prepn. of barbiturate-recognizing diphosphines and their macrocyclic palladium complexes as catalysts for auxiliary directed regioselective Heck arylation of alkenes)

RN 112817-57-9 HCAPLUS

CN 1,3-Benzenedicarboxamide, N,N'-bis(6-amino-2-pyridinyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 54 THERE ARE 54 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 32 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

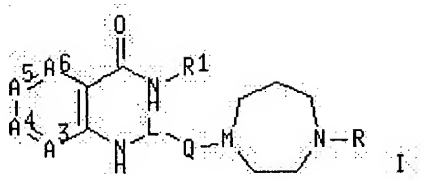
Full Text | CAPLUS References

ACCESSION NUMBER: 2002:637656 HCAPLUS
DOCUMENT NUMBER: 137:169553
TITLE: Preparation of substituted benzoylaminocarboxamides as inhibitors of factor Xa
INVENTOR(S): Herron, David Kent; Joseph, Sajan; Marquart, Angela Lynn; Masters, John Joseph; Mendel, David; Smith, Gerald Floyd; Waid, Philip Parker; Wiley, Michael Robert; Yee, Ying Kwong
PATENT ASSIGNEE(S): Eli Lilly and Company, USA
SOURCE: PCT Int. Appl., 116 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002064567	A2	20020822	WO 2001-US42941	20011114
WO 2002064567	C1	20031218		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
EP 1379506	A2	20040114	EP 2001-273729	20011114
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
US 2004058959	A1	20040325	US 2003-415756	20030430
PRIORITY APPLN. INFO.:			US 2000-253501P	P 20001128
			WO 2001-US42941	W 20011114

h eb c g cg b cg eb

OTHER SOURCE(S): MARPAT 137:169553
GI



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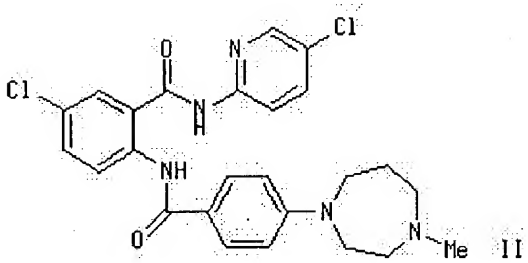


II

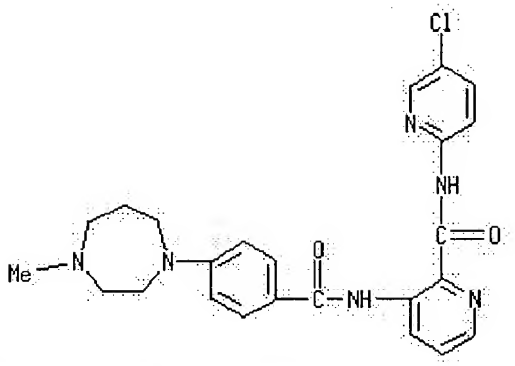
AB Title compds. I [R1 = (un)substituted 2-pyridinyl, 3-pyridinyl, Ph, 6-indolyl, 6-indazolyl; A3-6 together with the two carbons to which they are attached, complete a (un)substituted benzene, heteroarom., etc.; L = CO, methylene; M = N; Q = substituted Ph, cyclohexan-1,4-diyl, piperidin-1,4-diyl; R = H, alkyl, cycloalkyl, acyl, acetyloxyacetyl, aminoacetyl, hydroxyacetyl, alkoxycarbonyl, alkoxycarbonylmethyl, etc.] were prepd. For example, 5-Chloro-2-nitro-N-(5-chloropyridin-2-yl)benzamide (prepn. given) was reduced to the corresponding aniline (MeOH, NaBH4) and acylated with 4-fluorobenzoyl chloride (CH2Cl2, pyridine). This intermediate was reacted with 1-methylhexahydro-1,4-diazepine (DMSO, 90°, 24 h) to afford II. I are inhibitors of factor Xa and used to produce an anticoagulant or antithrombotic effect.

IT **448933-91-3P**, 3-[4-(4-Methylhexahydro-1,4-diazepin-1-yl)benzoylamino]-N-(5-chloropyridin-2-yl)pyridine-2-carboxamide
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(factor Xa inhibitor; prepn. of substituted benzoylaminocarboxamides as inhibitors of factor Xa)

RN 448933-91-3 HCAPLUS

CN 2-Pyridinecarboxamide, N-(5-chloro-2-pyridinyl)-3-[[4-(hexahydro-4-methyl-1H-1,4-diazepin-1-yl)benzoyl]amino]- (9CI) (CA INDEX NAME)

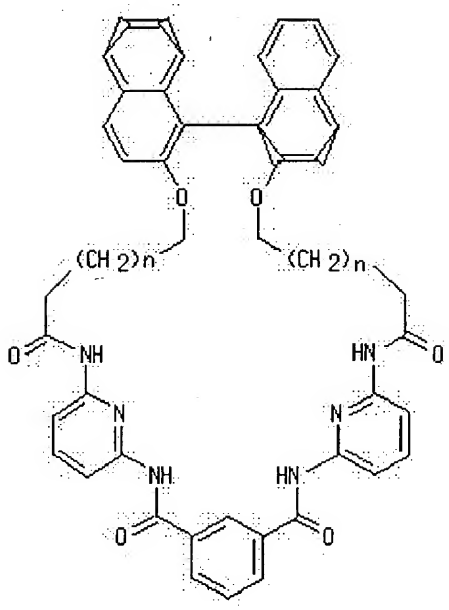
h eb c g cg b cg eb



L12 ANSWER 33 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 2002:517330 HCAPLUS
DOCUMENT NUMBER: 138:89785
TITLE: Synthesis and binding properties of chiral macrocyclic barbiturate receptors: application to nitrile oxide cyclizations
AUTHOR(S): Rasmussen, Brian S.; Elezcano, Unai; Skrydstrup, Troels
CORPORATE SOURCE: Department of Chemistry, University of Aarhus, Aarhus, 8000, Den.
SOURCE: Journal of the Chemical Society, Perkin Transactions 1 (2002), (14), 1723-1733
CODEN: JCSPCE; ISSN: 1472-7781
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:89785
GI



I

AB A series of chiral macrocyclic receptors I [n = 0-2, R = H; n = 3, R =

h eb c g cg b cg eb

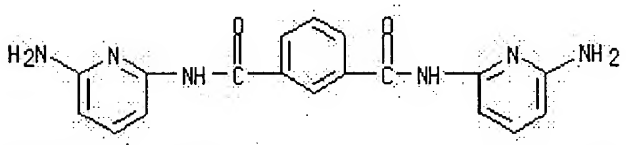
2-naphthyl], contg. a barbiturate binding domain, has been synthesized with the purpose of exploiting these for asym. 1,3-dipolar cycloaddns. Analogs with a modified deoxycholate moiety were similarly prepd. All the hosts with the exception of one effectively bind a barbiturate-cinnamic acid conjugate with assocn. consts. in the order of 104 M-1 in CDCl3. The 1,3-dipolar cycloaddn. between several arylnitrile oxides and the cinnamate conjugates were examd. in the presence of stoichiometric amts. of a chiral receptor affording two regioisomeric isoxazolines. Enantiomeric excesses of up to 30% were obtained in one case for the major regioisomer. In most cases, the enantiomeric excesses could be measured directly from the crude 1H-NMR spectra owing to the diastereomeric interaction between the isoxazoline cycloadduct and the chiral receptor. The relatively low enantiofacial selectivities at the C:C double bond of the cinnamate were attributed to the non-planar orientation of the barbiturate-cinnamate conjugate with respect to the receptor, as previously noted for the binding of barbital to an achiral macrocyclic host, directing the cinnamate unit away from the chiral unit.

IT **112817-57-9**

RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of macrocyclic barbiturate-contg. receptors as catalysts for asym. nitrile oxide cyclizations)

RN 112817-57-9 HCAPLUS

CN 1,3-Benzenedicarboxamide, N,N'-bis(6-amino-2-pyridinyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 64 THERE ARE 64 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 34 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 2002:428907 HCAPLUS
DOCUMENT NUMBER: 137:6180
TITLE: Preparation of 1,4,5,6-tetrahydroimidazo[4,5-d]benzazepine derivatives as vasopressin antagonists
INVENTOR(S): Koshio, Hiroyuki; Kakefuda, Akio; Sato, Ippei; Wakayama, Ryutaro; Sanagi, Masanao
PATENT ASSIGNEE(S): Yamanouchi Pharmaceutical Co., Ltd., Japan
SOURCE: PCT Int. Appl., 37 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002044179	A1	20020606	WO 2001-JP10328	20011127

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

h eb c g cg b cg eb

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

AU 2002024115	A5	20020611	AU 2002-24115	20011127
JP 2002226480	A2	20020814	JP 2001-361126	20011127
EP 1338597	A1	20030827	EP 2001-998171	20011127
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
US 2004034012	A1	20040219	US 2003-432732	20030527
PRIORITY APPLN. INFO.:			JP 2000-360809	A 20001128
			WO 2001-JP10328	W 20011127

OTHER SOURCE(S): MARPAT 137:6180

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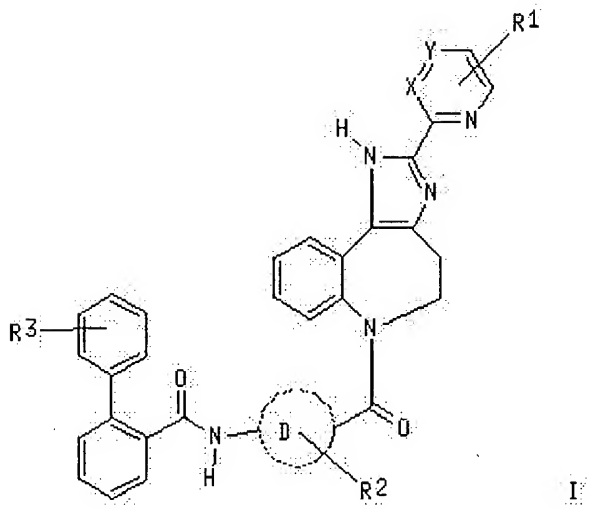


I

AB The title compds. I [ring D = phenylene, etc.; X, Y = CH, N; R1 - R3 = H, halo, etc.] are prepd. In an in vitro V1A receptor binding assay, compds. of this invention showed the pKi values of 8.12 to 8.71.

IT **433263-38-8P**

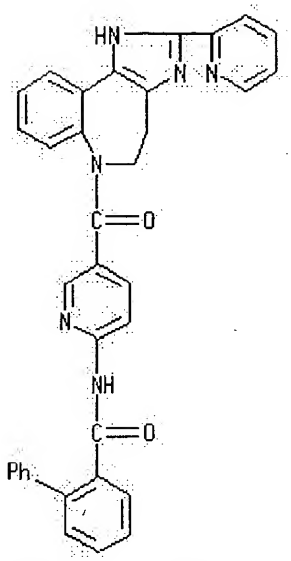
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of tetrahydroimidazobenzazepine derivs. as vasopressin antagonists)

RN 433263-38-8 HCAPLUS

CN [1,1'-Biphenyl]-2-carboxamide, N-[5-[[4,5-dihydro-2-(2-pyridinyl)imidazo[4,5-d][1]benzazepin-6(1H)-yl]carbonyl]-2-pyridinyl]-, monohydrochloride (9CI) (CA INDEX NAME)

h eb c g cg b cg eb



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REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 35 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

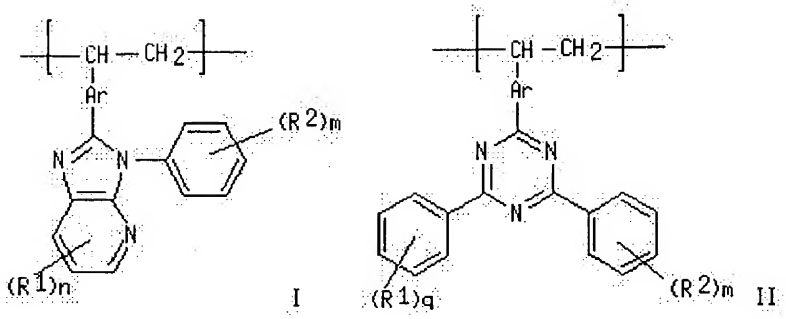
Full Text | Citing References

ACCESSION NUMBER: 2002:354001 HCAPLUS
DOCUMENT NUMBER: 136:377202
TITLE: Light-emitting device and material therefor
INVENTOR(S): Okada, Hisashi; Ise, Toshihiro; Mishima, Masayuki; Taguchi, Toshiki
PATENT ASSIGNEE(S): Fuji Photo Film Co., Ltd., Japan
SOURCE: U.S. Pat. Appl. Publ., 91 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
US 2002055014	A1	20020509	US 2001-935711		20010824
JP 2002319491	A2	20021031	JP 2001-236419		20010803
PRIORITY APPLN. INFO.:			JP 2000-254171	A	20000824
			JP 2001-38718	A	20010215
			JP 2001-236419	A	20010803

OTHER SOURCE(S): MARPAT 136:377202
GI

h eb c g cg b cg eb

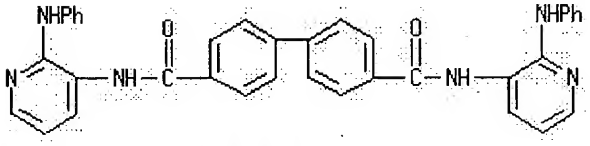


AB Light-emitting devices comprising a pair of electrodes formed on a substrate and org. compd. layers comprising a light-emitting layer provided in between the electrodes are described in which ≥1 of the org. compd. layers comprises a heterocyclic compd. having ≥2 atoms and a phosphorescent compd.; polymers with repeating units described by the general formulas I and II (Ar = arylene or divalent heterocyclic group; R1 and R2 = independently selected H or substituent; n = 0-3; q = 0-5; and m = 0-5), which may be employed as the heterocyclic compds. in the devices, are also described. The devices may also employ polymers of heterocyclic compds. from which AR is absent. The phosphorescent compd. may be an org. metal complex.

IT **377092-01-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(light-emitting devices with emitting layers including heterocyclic compds. and phosphorescent materials and heterocycle deriv. polymers for them)

RN 377092-01-8 HCAPLUS

CN [1,1'-Biphenyl]-4,4'-dicarboxamide, N,N'-bis[2-(phenylamino)-3-pyridinyl]- (9CI) (CA INDEX NAME)



L12 ANSWER 36 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER:	2002:275966 HCAPLUS
DOCUMENT NUMBER:	136:294739
TITLE:	Preparation of pyridinyl-substituted benzamides as Apo B secretion inhibitors
INVENTOR(S):	Takasugi, Hisashi; Terasawa, Takeshi; Inoue, Yoshikazu; Nakamura, Hideko; Nagayoshi, Akira; Ohtake, Hiroaki; Furukawa, Yoshiro; Mikami, Masafumi; Hinoue, Kazumasa; Ohtsubo, Makoto
PATENT ASSIGNEE(S):	Fujisawa Pharmaceutical Co., Ltd., Japan; Daiso Co., Ltd.
SOURCE:	PCT Int. Appl., 266 pp. CODEN: PIXXD2
DOCUMENT TYPE:	Patent
LANGUAGE:	English
FAMILY ACC. NUM. COUNT:	1

PATENT INFORMATION:

h eb c g cg b cg eb

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002028835	A1	20020411	WO 2001-JP8581	20010928
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2001092315	A5	20020415	AU 2001-92315	20010928
EP 1326835	A1	20030716	EP 2001-972612	20010928
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
BR 2001014657	A	20030930	BR 2001-14657	20010928
JP 2004510763	T2	20040408	JP 2002-532421	20010928
NZ 525591	A	20040430	NZ 2001-525591	20010928
NO 2003001540	A	20030605	NO 2003-1540	20030404
US 2004058903	A1	20040325	US 2003-381737	20030903
PRIORITY APPLN. INFO.:			AU 2000-583 A	20001005
			AU 2001-6666 A	20010727
			WO 2001-JP8581 W	20010928

OTHER SOURCE(S): MARPAT 136:294739

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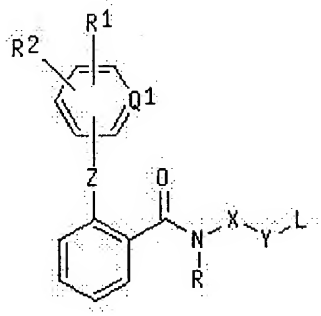

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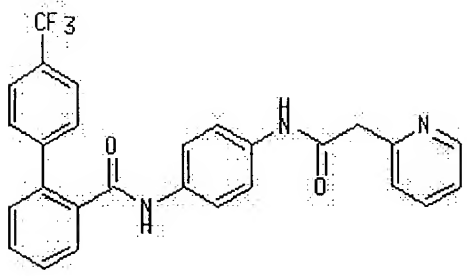

II

AB Title compds. I [wherein R1 and R2 = independently alkyl, alkenyl, acyl, amino, (cyclo)alkoxy, aryl(oxy), sulfoxy, mercapto, sulfo, H, halo, NO2, CN, or OH; or R1R2 = a ring; Q1 = N or CH; L = (un)substituted unsatd. 3 to 10-membered heterocyclic group; X = (un)substituted monocyclic (hetero)arylene; Y = (A1)m(A2)n(A4)k; Z = direct bond, CH2, NH, or O; R = H or alkyl; A1 = (un)substituted alkylene or alkenylene; A2 = NR3, CONR3, NHCONH, CO2, O, O(CH2)2NR3, S, SO, or SO2; A4 = alkylene, alkenylene, or alkynylene; R3 = H or suitable substituent; k, m, and m = independently 0 or 1; or a salt thereof] were prepd. as apolipoprotein B (Apo B) secretion

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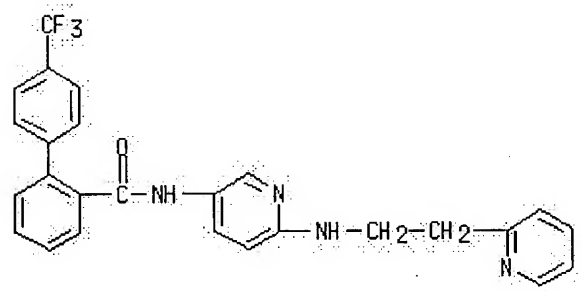
inhibitors. For example, to a suspension of N-(4-aminophenyl)-4'-(trifluoromethyl)-1,1'-biphenyl-2-carboxamide, 2-pyridinylacetic acid•HCl, and HOBT•H2O in CH2Cl2 was added to WSC•HCl, followed by TEA at 5°C. The mixt. was stirred at room temp. for 24 h and worked up to give II. The latter inhibited Apo B secretion by 100% at 10-6 M in HepG2 cells and lowered cholesterol by 83% and triglyceride by 35% after 2 h at a dose of 32 mg/kg in ddY-mice. I are useful for the prophylaxis and treatment of diseases or conditions resulting from elevated circulating levels of Apo B, such as hyperlipemia, hyperlipidemia, hyperlipoproteinemia, hypoalphalipoproteinemia, hypercholesterolemia, hypertriglyceridemia, atherosclerosis, pancreatitis, non-insulin dependent diabetes mellitus, obesity, coronary heart diseases, myocardial infarction, stroke, restenosis, and Syndrome X.

IT **366488-08-6P**, N-[6-[[2-(2-Pyridinyl)ethyl]amino]-3-pyridinyl]-4'-(trifluoromethyl)-1,1'-biphenyl-2-carboxamide
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(Apo B inhibitor; prepn. of pyridinyl-substituted benzamides as Apo B secretion inhibitors for treatment of obesity, NIDDM, and related conditions)

RN 366488-08-6 HCAPLUS

CN [1,1'-Biphenyl]-2-carboxamide, N-[6-[[2-(2-pyridinyl)ethyl]amino]-3-pyridinyl]-4'-(trifluoromethyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 37 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 2002:237687 HCAPLUS
DOCUMENT NUMBER: 137:11116
TITLE: Steady-State Concentration Distribution of Artificial Receptor and Target Analyte in Plasticized PVC Membrane between Solutions Differing in Target Analyte Concentration
AUTHOR(S): Zhang, Xu; Zhao, Hong; Weber, Stephen G.
CORPORATE SOURCE: Department of Chemistry, University of Pittsburgh, Pittsburgh, PA, 15260, USA
SOURCE: Analytical Chemistry (2002), 74(9), 2184-2189
CODEN: ANCHAM; ISSN: 0003-2700
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A barbiturate receptor was proven effective in improving selectivity in solid-phase microextn. of barbiturates when doped into plasticized poly(vinyl chloride) (PVC). It would be beneficial to have selective extns. for any given org. species; however, the receptors do not exist.

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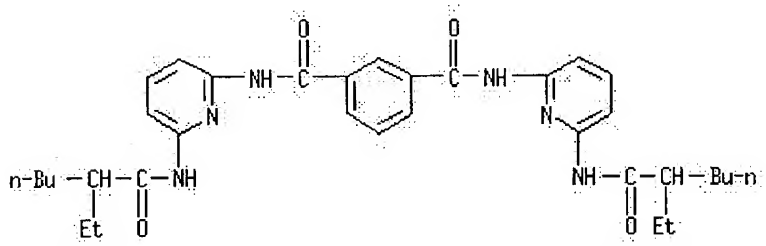
They will be found by screening of libraries of potential receptors; thus, a screening method was needed. It is important to screen the receptors in the medium in which they will work: plasticized PVC. We hypothesize that we can make receptors move in soln. in response to the presence of a solute to which they bind. This work examines whether we can establish a sufficient free energy gradient for a good receptor to move to a predetd. place in space. A difference in the barbiturate solute (substrate or guest) concn. in solns. bathing the two sides of a plasticized PVC membrane contg. the barbiturate receptor (or host) creates a spatial concn. gradient of the substrate in the membrane. This causes the receptor's chem. potential to vary across the membrane. Upon binding to the analyte, the receptor undergoes a local activity drop, which decreases its free energy. This process produces a flux of receptor to accumulate at place where there was a high substrate concn. A concn. gradient of substrate can be maintained across the membrane at steady state. In membranes for which the formation of the complex was favored, the receptor responds to the gradient of substrate. In membranes for which binding is not favored, a gradient of substrate was completely ignored by the receptor. Thus, the receptor does respond to the gradient but only if the concn. gradient of guest corresponds to a chem. potential gradient.

IT 228271-35-0
RL: ANT (Analyte); ANST (Analytical study)
(phenobarbital receptor; steady-state concn. distribution of artificial receptor and target analyte in plasticized PVC membrane between solns. differing in target analyte concn.)

RN 228271-35-0 HCAPLUS

CN 1,3-Benzenedicarboxamide, N,N'-bis[6-[(2-ethyl-1-oxohexyl)amino]-2-pyridinyl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 38 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 2002:225542 HCAPLUS
DOCUMENT NUMBER: 137:6501
TITLE: Supramolecular polymers generated from heterocomplementary monomers linked through multiple hydrogen-bonding arrays-formation, characterization, and properties
AUTHOR(S): Berl, Volker; Schmutz, Marc; Krische, Michael J.; Khoury, Richard G.; Lehn, Jean-Marie
CORPORATE SOURCE: Laboratoire de Chimie Supramoleculaire, ESA 7006 of the CNRS, ISIS, Universite Louis Pasteur, Strasbourg, 67000, Fr.
SOURCE: Chemistry--A European Journal (2002), 8(5), 1227-1244
CODEN: CEUJED; ISSN: 0947-6539
PUBLISHER: Wiley-VCH Verlag GmbH
DOCUMENT TYPE: Journal
LANGUAGE: English

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AB Supramol. polymers are described that are derived from the assocn. of two homoditopic heterocomplementary monomers through sextuple hydrogen-bonding arrays. They form fibers and a variety of different materials depending on the conditions. The strong affinity of the DAD - DAD (D=donor, A=acceptor) hydrogen-bonding sites for double-faced cyanuric acid type wedges drives the supramol. polymeric assembly in apolar and chlorinated org. solvents. The marked influence of stoichiometry, as well as end-capping and crosslinking agents upon fiber formation is revealed in soln. and by electron microscopy (EM). The results further contribute to the development of a supramol. polymer chem. that comprizes reversible polymers formed through recognition-controlled noncovalent connections between the mol. components. Such materials are, by nature, dynamic and present adaptive character in view of their ability to respond to external stimuli.

IT **433216-82-1P**

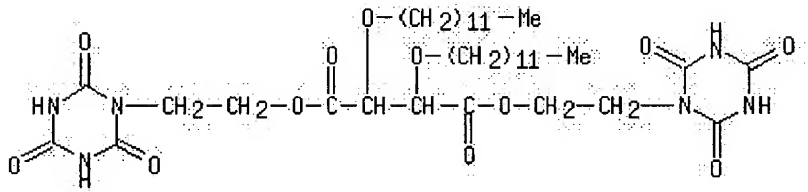
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (polymers from heterocomplementary monomers linked through multiple hydrogen-bonding arrays)

RN 433216-82-1 HCAPLUS

CN Butanedioic acid, 2,3-bis(dodecyloxy)-, bis[2-(tetrahydro-2,4,6-trioxo-1,3,5-triazin-1(2H)-yl)ethyl] ester, polymer with 5,5'-[1,3-propanediylbis(oxy)]bis[N,N'-bis[6-[(1-oxobutyl)amino]-2-pyridinyl]-1,3-benzenedicarboxamide] (9CI) (CA INDEX NAME)

CM 1

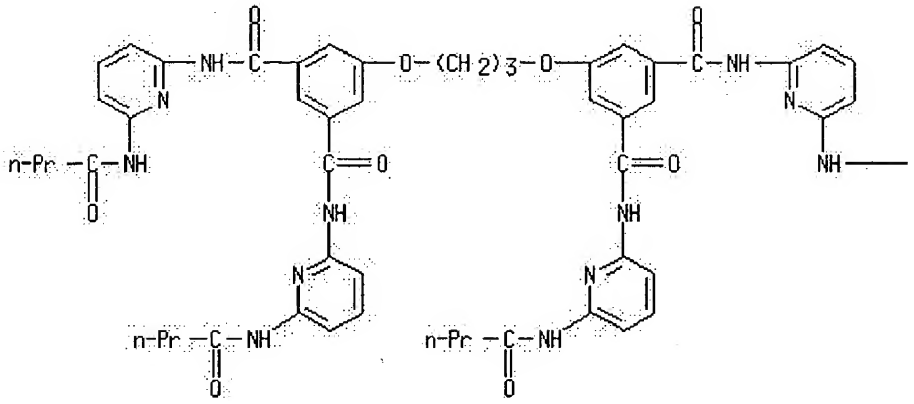
CRN 433216-81-0
CMF C38 H64 N6 O12



CM 2

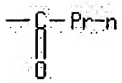
CRN 433216-79-6
CMF C55 H60 N12 O10

PAGE 1-A



h eb c g cg b cg eb

PAGE 1-B



REFERENCE COUNT: 83 THERE ARE 83 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 39 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

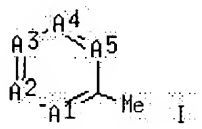
Full Text | CITED References

ACCESSION NUMBER: 2002:169229 HCAPLUS
DOCUMENT NUMBER: 136:224165
TITLE: Silver halide color photographic light-sensitive film exhibiting low fogging
INVENTOR(S): Kataoka, Emiko; Kagawa, Nobuaki; Tanaka, Tatsuo
PATENT ASSIGNEE(S): Konica Corporation, Japan
SOURCE: Eur. Pat. Appl., 71 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1184717	A2	20020306	EP 2001-121093	20010903
EP 1184717	A3	20020807		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
JP 2002148750	A2	20020522	JP 2000-349538	20001116
US 2002081543	A1	20020627	US 2001-942402	20010830
US 6566043	B2	20030520		

PRIORITY APPLN. INFO.: JP 2000-266877 A 20000904
JP 2000-349538 A 20001116

OTHER SOURCE(S): MARPAT 136:224165
GI

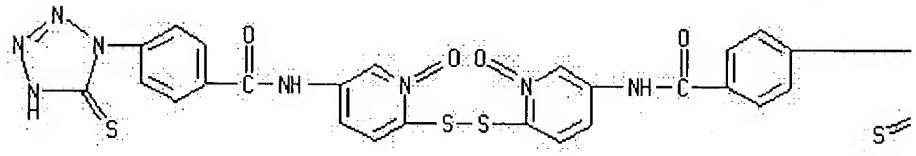


AB The present invention provides a silver halide photog. light-sensitive film comprising a support having thereon a light-sensitive silver halide emulsion layer comprising a compd. represented by the formula Z-S-X ; wherein Z = group represented by the Formula I (A1, A2, A3, A4, A5 each represent =N-, =N(→O)-, and substituents further defined in the claims), X = H, or Z-S-. The object of the present invention is to provide a silver halide photog. light-sensitive film, comprising mercapto compds. and disulfide compds., which exhibits low fogging, excellent pressure resistance, and excellent sensitivity.

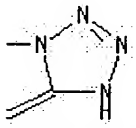
h eb c g cg b cg eb

IT 402726-48-1
RL: TEM (Technical or engineered material use); USES (Uses)
(fog inhibitor; silver halide color photog. light-sensitive film exhibiting low fogging)
RN 402726-48-1 HCAPLUS
CN Benzamide, N,N'-[dithiobis(1-oxido-2,5-pyridinediyl)]bis[4-(2,5-dihydro-5-thioxo-1H-tetrazol-1-yl)- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B



L12 ANSWER 40 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Other References

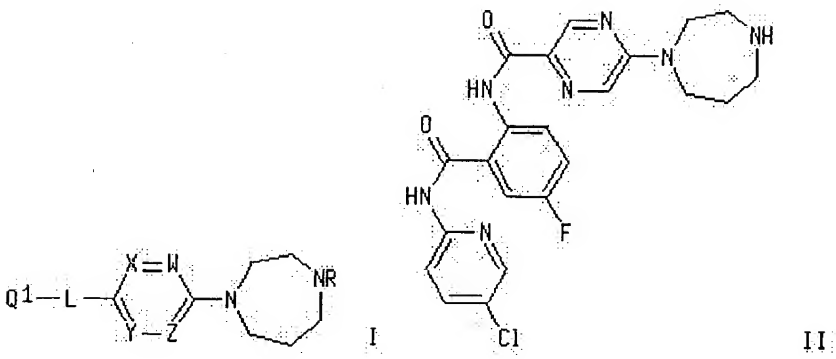
ACCESSION NUMBER: 2002:107335 HCAPLUS
DOCUMENT NUMBER: 136:151189
TITLE: Preparation of pyrazinyl-, pyridazinyl-, pyrimidinyl-, and pyridinyl-hexahydrodiazepines and their use as factor Xa inhibitors
INVENTOR(S): Herron, David Kent; Joseph, Sajan; Marquart, Angela Lynn; Masters, John Joseph; Mendel, David; Smith, Gerald Floyd; Waid, Philip Parker; Wiley, Michael Robert; Yee, Ying Kwong
PATENT ASSIGNEE(S): Eli Lilly and Company, USA
SOURCE: PCT Int. Appl., 159 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002010154	A2	20020207	WO 2001-US16528	20010718
WO 2002010154	A3	20020627		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
EP 1307444	A2	20030507	EP 2001-958825	20010718
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
US 2004097491	A1	20040520	US 2003-332120	20030102

h eb c g cg b cg eb

PRIORITY APPLN. INFO.: US 2000-221092P P 20000727
WO 2001-US16528 W 20010718

OTHER SOURCE(S): MARPAT 136:151189
GI

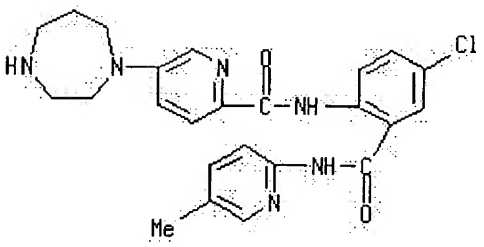


AB Substituted hexahydrodiazepines I [R = H, alkyl, acyl, acetyloxy, acetyl, aminoacetyl, alkylamido, etc.; one or two of X, W, Y, and Z equals N and each of the others of X, W, Y and Z is CH; when L = CO or CH2, Q1 = (un)substituted pyridinyl- or phenyl-amidophenylamine, in addn. when L = CO, Q1 may equal Q2X2SO2N(CH2CH2)2N- wherein Q2 = (un)substituted Ph, benzo[b]thiophen-2-yl or naphthalen-2-yl (X2 = direct bond, CH2, ethylene, or ethen-1,2-diyl)], and their pharmaceutically acceptable salts are prepd. and disclosed as factor Xa inhibitors. Thus, II was prepd. by amidation of 2-amino-5-fluoro-N-(5-chloropyridin-2-yl)benzamide with 5-hydroxy-pyrazine-2-carboxylic acid (via its acid chloride) followed by substitution with 1-BOC-hexahydro-1,4-diazepine and subsequent deprotection of the diazepinyl nitrogen. As factor Xa inhibitors, the compds. of the invention are claimed to be useful in the treatment of thromboembolic disorders (no data).

IT **395683-78-0P**
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(prepn. of pyrazinyl-, pyridazinyl-, pyrimidinyl-, and pyridinyl-hexahydrodiazepines as factor Xa inhibitors)

RN 395683-78-0 HCAPLUS

CN 2-Pyridinecarboxamide, N-[4-chloro-2-[[(5-methyl-2-pyridinyl)amino]carbonyl]phenyl]-5-(hexahydro-1H-1,4-diazepin-1-yl)- (9CI) (CA INDEX NAME)



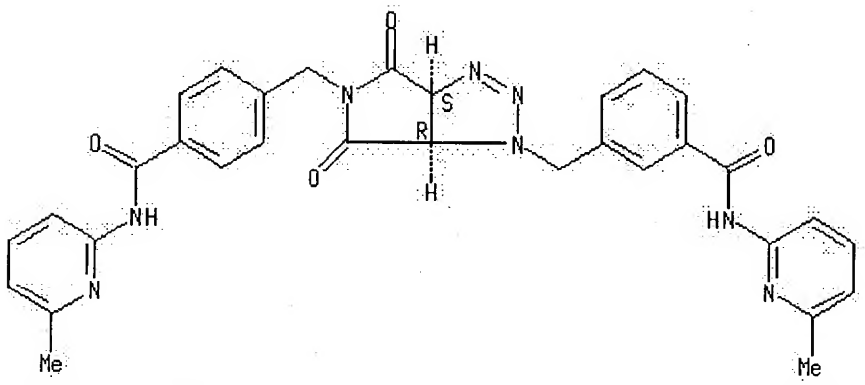
L12 ANSWER 41 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

h eb c g cg b cg eb

ACCESSION NUMBER: 2002:14174 HCAPLUS
DOCUMENT NUMBER: 136:216362
TITLE: A Generic Recognition-Based Approach to the Acceleration of Cycloaddition Reactions
AUTHOR(S): Howell, Sarah J.; Spencer, Neil; Philp, Douglas
CORPORATE SOURCE: Centre for Biomolecular Sciences School of Chemistry, University of St. Andrews, St Andrews, KY16 9ST, UK
SOURCE: Organic Letters (2002), 4(2), 273-276
CODEN: ORLEF7; ISSN: 1523-7060
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Dicarboxylic acids accelerate the rate of cycloaddn. reactions between either an azide or a furan and a maleimide through the formation of a reactive 1:1:1 complex stabilized by four hydrogen bonds.
IT 402750-23-6
RL: FMU (Formation, unclassified); PRP (Properties); FORM (Formation, nonpreparative)
(recognition-based approach to acceleration of cycloaddn. reactions)
RN 402750-23-6 HCAPLUS
CN Benzamide, N-(6-methyl-2-pyridinyl)-3-[[(3aR,6aS)-4,5,6,6a-tetrahydro-5-[[4-[[(6-methyl-2-pyridinyl)amino]carbonyl]phenyl]methyl]-4,6-dioxopyrrolo[3,4-d]-1,2,3-triazol-1(3aH)-yl]methyl]-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT: 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 42 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN
Full Text | Cited References

ACCESSION NUMBER: 2002:11104 HCAPLUS
DOCUMENT NUMBER: 136:69743
TITLE: Preparation of pyridyl benzamides and related compounds as Factor Xa inhibitors.
INVENTOR(S): Zhu, Bing-Yan; Zhang, Penglie; Wang, Lingyan; Huang, Wenrong; Goldman, Erick A.; Li, Wenhao; Zuckett, Jingmei; Song, Yonghong; Scarborough, Robert
PATENT ASSIGNEE(S): USA
SOURCE: U.S. Pat. Appl. Publ., 259 pp., Cont.-in-part of U.S. Ser. No. 663,420.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 6

h eb c g cg b cg eb

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2002002183	A1	20020103	US 2001-794225	20010228
US 6376515	B2	20020423		
US 2003162690	A1	20030828	US 2002-126976	20020422
US 2004097561	A1	20040520	US 2003-687334	20031015
PRIORITY APPLN. INFO.:			US 2000-185746P	P 20000229
			US 2000-663420	A2 20000915
			US 2001-794225	A1 20010228
			US 2002-126976	A1 20020422

OTHER SOURCE(S): MARPAT 136:69743

AB AQDEGJX [A = alkyl, cycloalkyl, NR1R2, NR1R2C(:NR3), (substituted) Ph, naphthyl, heterocyclyl, etc.; R1-R3 = H, OR5, NR5R6, alkyl, alkenyl, etc.; R1R2 or R2R3 = atoms to form (substituted) cycloalkyl, heterocyclyl; R5, R6 = H, alkyl, alkenyl, alkynyl, cycloalkyl, (substituted) alkylphenyl, alkylnaphthyl; R5R6 = atoms to form a 3-8 membered (substituted) ring; Q = bond, CH2, CO, O, S, SO, SO2, NR7, SO2NR7, etc.; R7 = H, alkyl, alkenyl, alkynyl, cycloalkyl, alkylcycloalkyl, (substituted) alkylphenyl, alkylnaphthyl; D = bond, (substituted) Ph, naphthyl, mono- or bicyclic heterocyclyl; E = bond, alkyl, O, S, SO, SO2, alkylcarbonyl, etc.; G = (substituted) alkenyl, cycloalkenyl, phenylene, 3-8 membered (fused) (arom.) heterocyclyl; J = bond, NR9CO, O, S, SO, SO2, CH2, NR9SO2, etc.; X = (substituted) Ph, naphthyl, (fused) heteroaryl], were prepd. as antithrombotics (no data). Thus, N-(5-bromo-2-pyridinyl)-2-aminophenylcarboxamide (prepn. given), 4-cyanobenzoyl chloride, and pyridine were stirred overnight in CH2Cl2 to give 70% N-(5-bromo-2-pyridinyl)-[2-(4-cyanophenylcarbonyl)amino]phenylcarboxamide. The latter in MeOH at 0° was satd. with HCl and stirred overnight followed by solvent evapn. The residue was refluxed 2 h with NH4OAc in MeOH to give 70% N-(5-bromo-2-pyridinyl)-[2-(4-amidinophenylcarbonyl)amino]phenylcarboxamide.

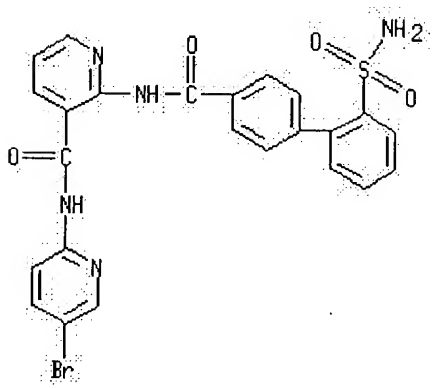
IT **330939-74-7P**

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of pyridyl benzamides and related compds. as Factor Xa inhibitors)

RN 330939-74-7 HCAPLUS

CN 3-Pyridinecarboxamide, 2-[[[2'-(aminosulfonyl)[1,1'-biphenyl]-4-yl]carbonyl]amino]-N-(5-bromo-2-pyridinyl)- (9CI) (CA INDEX NAME)



L12 ANSWER 43 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

h eb c g cg b cg eb

Full Text | Citing References

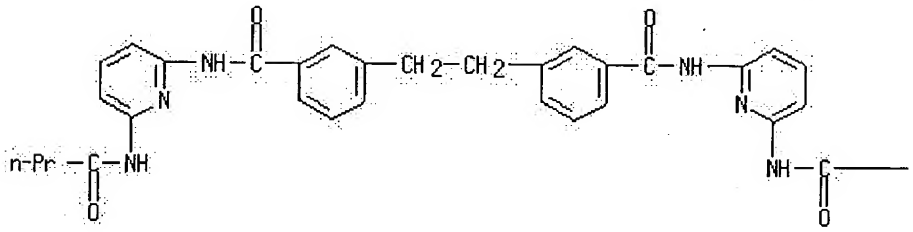
ACCESSION NUMBER: 2001:896753 HCAPLUS
DOCUMENT NUMBER: 136:118326
TITLE: Molecular recognition of xanthine alkaloids: first synthetic receptors for theobromine and a series of new receptors for caffeine
AUTHOR(S): Goswami, Shyamaprosad; Mahapatra, Ajit Kumar; Mukherjee, Reshmi
CORPORATE SOURCE: Department of Chemistry, Bengal Engineering College (Deemed University), Howrah, 711103, India
SOURCE: Journal of the Chemical Society, Perkin Transactions 1 (2001), (20), 2717-2726
CODEN: JCSPCE; ISSN: 1472-7781
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 136:118326
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Synthetic receptors [I, II (R = H, Ac) and III] are designed and synthesized for the first time for theobromine, a xanthine alkaloid used as a diuretic. The synthesis of the receptor III is achieved by Co(PPh3)3Cl-mediated homocoupling of 3-(ethoxycarbonyl)benzyl bromide under mild conditions. New caffeine receptors [IV and V (X = CH2, SO2)] are designed and synthesized. The binding results of theobromine and caffeine (both by NMR and UV studies) are reported.

IT **390358-50-6P**
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PYP (Physical process); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); PROC (Process); RACT (Reactant or reagent)
(mol. recognition of xanthine alkaloids by synthetic receptors specific for theobromine or caffeine)
RN 390358-50-6 HCAPLUS
CN Benzamide, 3,3'-(1,2-ethanediyl)bis[N-[6-[(1-oxobutyl)amino]-2-pyridinyl]- (9CI) (CA INDEX NAME)

PAGE 1-A



h eb c g cg b cg eb

—Pr-n
REFERENCE COUNT: 39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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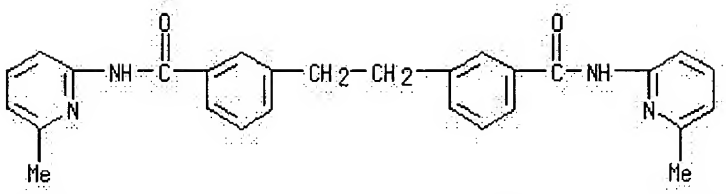
h eb c g cg b cg eb



REFERENCE COUNT: 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 73 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Other References

ACCESSION NUMBER: 2000:144899 HCAPLUS
DOCUMENT NUMBER: 132:189658
TITLE: Amino acid derivative and peptide anti-cancer compounds and methods
INVENTOR(S): Stewart, John M.; Chan, Daniel C. F.; Gera, Lojos; York, Eunice; Bunn, Paul
PATENT ASSIGNEE(S): USA
SOURCE: PCT Int. Appl., 55 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 2000011022	A1	20000302	WO 1999-US19381		19990820
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM					
RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG					
US 6388054	B1	20020514	US 1999-378019		19990819
AU 2000015959	A1	20000314	AU 2000-15959		19990820
US 2002183252	A1	20021205	US 2001-35662		20011228
PRIORITY APPLN. INFO.:			US 1998-97210P	P	19980820
			US 1999-141169P	P	19990625
			US 1999-378019	A	19990819
			WO 1999-US19381	W	19990820

OTHER SOURCE(S): MARPAT 132:189658

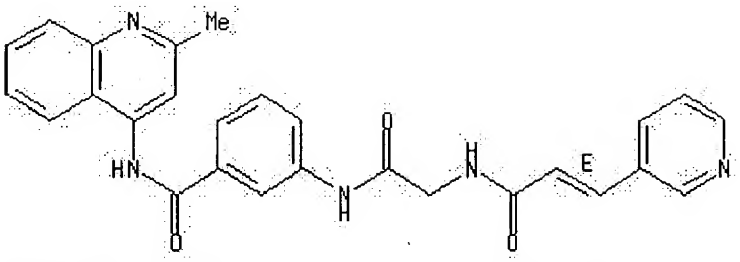
AB The invention provides amino acid deriv. and peptidic compds. useful to inhibit tumor growth and to induce apoptosis. In general, the anti-cancer agents (ACA) are described by the formula [ACA]n-X [X = linker group with 2-5 functional groups or is absent; n = 1; ACA as described in the invention (Markush included)].

IT **259885-31-9P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(peptide and non-peptide anti-cancer compds. and methods)

RN 259885-31-9 HCAPLUS
CN Benzamide, N-(2-methyl-4-quinolinyl)-3-[[[[(2E)-1-oxo-3-(3-pyridinyl)-2-propenyl]amino]acetyl]amino]- (9CI) (CA INDEX NAME)

h eb c g cg b cg eb

Double bond geometry as shown.

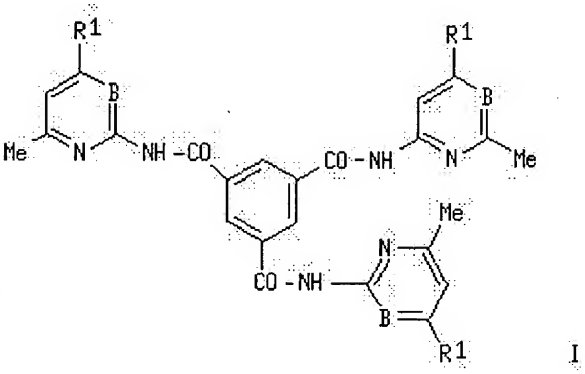


REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 74 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Other References

ACCESSION NUMBER: 2000:132410 HCAPLUS
DOCUMENT NUMBER: 132:293937
TITLE: Molecular recognition of carbohydrates by artificial polypyridine and polypyrimidine receptors
AUTHOR(S): Mazik, Monika; Bandmann, Heinz; Sicking, Willi
CORPORATE SOURCE: Institut fur Organische Chemie der Universitat Essen, Essen, 45117, Germany
SOURCE: Angewandte Chemie, International Edition (2000), 39(3), 551-554
CODEN: ACIEF5; ISSN: 1433-7851
PUBLISHER: Wiley-VCH Verlag GmbH
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

AB The recognition and binding of monosaccharides to simple, acyclic saccharide receptors, I (B = CH; R1 = H) and (B = N; R1 = Me), which incorporate three pyridine-amide or pyrimidine-amide moieties interconnected by a Ph spacer are discussed. Although these host mols. possess an acyclic structure, they are able to bind effectively to monosaccharides. These types of host mols. provide both hydrogen bonding sites and it-bonds for facilitating stacking interactions and thus participate in three-dimensional recognition of sugars.

IT 264626-71-3P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(mol. recognition of carbohydrates by artificial polypyridine and polypyrimidine receptors)

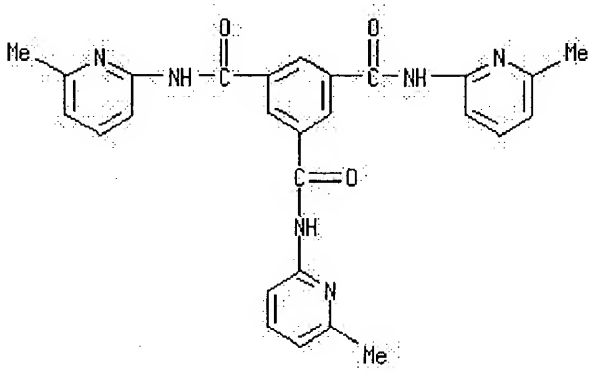
RN 264626-71-3 HCAPLUS

h eb c g cg b cg eb

CN β-D-Glucopyranoside, octyl, compd. with N,N',N''-tris(6-methyl-2-pyridinyl)-1,3,5-benzenetricarboxamide (1:1) (9CI) (CA INDEX NAME)

CM 1

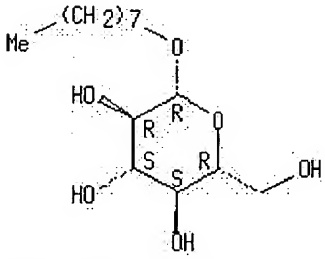
CRN 164174-81-6
CMF C27 H24 N6 O3



CM 2

CRN 29836-26-8
CMF C14 H28 O6

Absolute stereochemistry. Rotation (-).



REFERENCE COUNT: 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 75 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Cited References

ACCESSION NUMBER: 2000:63275 HCAPLUS
DOCUMENT NUMBER: 134:125538
TITLE: Three-dimensional quantitative structure-activity relationship study on cyclic urea derivatives as HIV-1 protease inhibitors: application of comparative molecular field analysis. [Erratum to document cited in CA130:217600]
AUTHOR(S): Debnath, Asim Kumar
CORPORATE SOURCE: Biochemical Virology Laboratory, Lindsley F. Kimball Research, Institute of The New York Blood Center, New York, NY, 10021, USA
SOURCE: Journal of Medicinal Chemistry (2000), 43(4), 764
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

h eb c g cg b cg eb

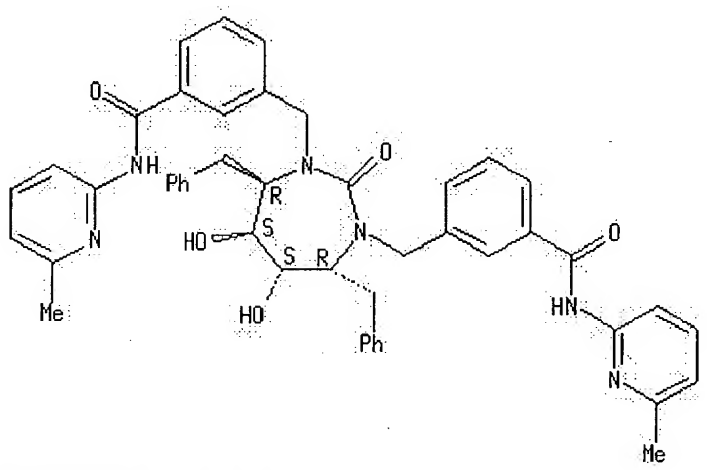
AB The last two structures representing compds. 104-118 are incorrect; the correct structure is given.

IT **183854-97-9**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(QSAR study on cyclic urea derivs. as HIV-1 protease inhibitors: application of comparative mol. field anal. (Erratum))

RN 183854-97-9 HCAPLUS

CN Benzamide, 3,3'-[[(4R,5S,6S,7R)-tetrahydro-5,6-dihydroxy-2-oxo-4,7-bis(phenylmethyl)-1H-1,3-diazepine-1,3(2H)-diyl]bis(methylene)]bis[N-(6-methyl-2-pyridinyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L12 ANSWER 76 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

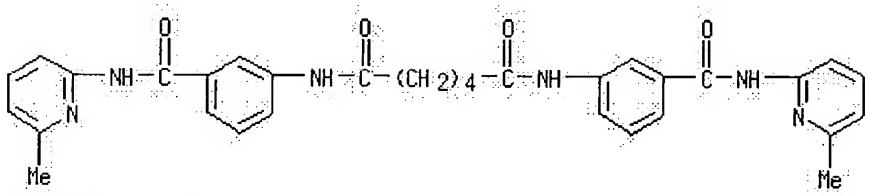
ACCESSION NUMBER:	2000:46405 HCAPLUS
DOCUMENT NUMBER:	132:194631
TITLE:	Three-point hydrogen bondings of carboxyl group in recognition of carboxylic acid and amino acid with designed synthetic receptors
AUTHOR(S):	Goswami, Shyamaprosad; Ghosh, Kumaresh; Mukherjee, Reshmi
CORPORATE SOURCE:	Department of Chemistry, Bengal Engineering College, Deemed University, Howrah, 711 103, India
SOURCE:	Journal of the Indian Chemical Society (1999), 76(11-12), 661-664 CODEN: JICSAH; ISSN: 0019-4522
PUBLISHER:	Indian Chemical Society
DOCUMENT TYPE:	Journal
LANGUAGE:	English
GI	

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The binding of carboxylic acids and amino acids were reported with designed synthetic receptors. The 3-point binding of carboxylic acids (with receptors I-III) was used to bind acetylglycine with receptor 6.

h eb c g cg b cg eb

IT **259728-69-3P**
RL: PEP (Physical, engineering or chemical process); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); PROC (Process); RACT (Reactant or reagent)
(three-point hydrogen bondings of carboxyl group in recognition of carboxylic acid and amino acid with designed synthetic receptors)
RN 259728-69-3 HCAPLUS
CN Hexanediamide, N,N'-bis[3-[[(6-methyl-2-pyridinyl)amino]carbonyl]phenyl]-(9CI) (CA INDEX NAME)



REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 77 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 1999:784096 HCAPLUS
DOCUMENT NUMBER: 132:12266
TITLE: Preparation of N-acylarylalanines as α4 integrin antagonists
INVENTOR(S): Head, John Clifford; Warrelow, Graham John; Porter, John Robert; Archibald, Sarah Catherine
PATENT ASSIGNEE(S): Celltech Therapeutics Limited, UK
SOURCE: PCT Int. Appl., 47 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9962901 A1		19991209	WO 1999-GB1741	19990603

W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG

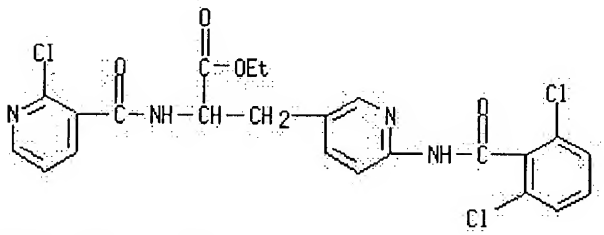
PRIORITY APPLN. INFO.: GB 1998-11969 19980603
OTHER SOURCE(S): MARPAT 132:12266
GI For diagram(s), see printed CA Issue.
AB R1Z1ZZ2Z3CRR4R5 [I; R = CO2 or deriv. thereof (sic); R1 = H, (hetero)cycloaliph. group, (hetero)aryl; R4 = H or Me; R5 = NHCOR6, NHCSR6, etc.; R6 = (hetero)(cyclo)aliph. group, (hetero)aryl, etc.; Z = bond or linker atom or group (sic); Z1 = bond, divalent (hetero)aliph. group; Z2 = pyridinediyl, pyrimidinediyl, pyrazinediyl, etc.; Z3 = bond or alkylene] were prepd. Thus, Ph2CHNHCH2CO2Et was alkylated by 2-bromomethyl-5-phenylsulfonyloxypyridine and the N-deprotected product acylated by N-acetyl-D-thioproline to give, after sapon., a diastereomeric mixt. of title compd. II. Data for biol. activity of I were given.
IT **251458-86-3P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological

h eb c g cg b cg eb

study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of N-acylarylalanines as α4 integrin antagonists)

RN 251458-86-3 HCAPLUS

CN 3-Pyridinepropanoic acid, α-[[(2-chloro-3-pyridinyl)carbonyl]amino]-6-[(2,6-dichlorobenzoyl)amino]-, ethyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 78 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 1999:779251 HCAPLUS
DOCUMENT NUMBER: 132:20807
TITLE: Self-assembling, chromogenic receptors for the recognition of medically important substrates and their method of use
INVENTOR(S): Goodman, M. Scott; Hamilton, Andrew D.
PATENT ASSIGNEE(S): University of Pittsburgh of the Commonwealth System of Higher Education, USA
SOURCE: U.S., 21 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5998594	A	19991207	US 1994-368209	19941230

PRIORITY APPLN. INFO.: US 1994-368209 19941230

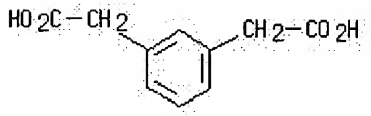
AB A chromogenic receptor comprises a self-assembled chromogenic compd. having at least one intrinsic binding site. The chromogenic compd. is characterized by the property of producing a reversible color change responsive to binding a target substrate to the receptor. The chromogenic compd. has a transition metal ion and at least one ligand bound to the transition metal ion. The ligand is selected from the group consisting of substituted phenanthroline, substituted 2,2'-bipyridine and substituted 2,2':6',2"-terpyridine. The transition metal is selected from the group consisting of Cu(I), Cu(II), Ag(I), Ni(II), Fe(II), Fe(III), Ru(II), Co(III), and Os(II). Self-assembly can be effected in the presence of Cu(I) to form receptors for dicarboxylic acids, carbohydrate, amino acids, steroids and pyrophosphates. The receptors are characterized by the formation of a 2:1 complex of the target substrate with the receptor producing a visible color change from orange to red and a measurable change in its luminescence. Methods of using these receptors are also disclosed.

IT 167496-61-9
RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses)
(self-assembling, chromogenic receptors for recognition of medically

important substrates and method of use)
RN 167496-61-9 HCAPLUS
CN Copper(1+), bis[4,4'-(1,10-phenanthroline-2,9-diyl-κN1,κN10)bis[N-(6-methyl-2-pyridinyl)benzamide]]-, (T-4)-, tetrafluoroborate(1-), 1,3-benzenediacetate (1:2) (9CI) (CA INDEX NAME)

CM 1

CRN 19806-17-8
CMF C10 H10 O4



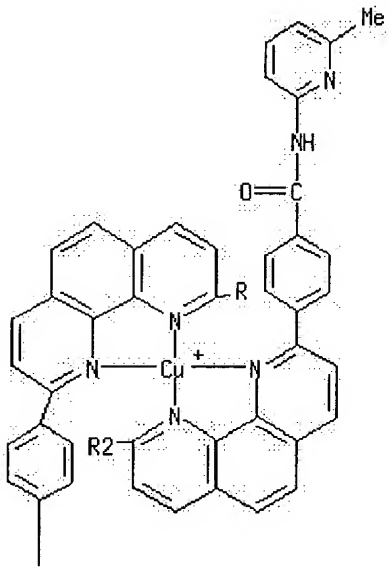
CM 2

CRN 167496-54-0
CMF C76 H56 Cu N12 O4 . B F4

CM 3

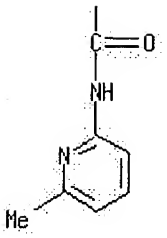
CRN 167496-53-9
CMF C76 H56 Cu N12 O4
CCI CCS

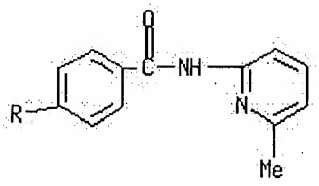
PAGE 1-A



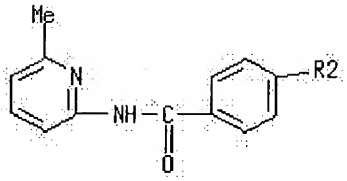
h eb c g cg b cg eb

PAGE 2-A



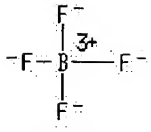


PAGE 3-A



CM 4

CRN 14874-70-5
CMF B F4
CCI CCS



REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 79 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 1999:733987 HCAPLUS
DOCUMENT NUMBER: 132:44883
TITLE: Induced fit selection of a barbiturate receptor from a dynamic structural and conformational/configurational library
AUTHOR(S): Berl, Volker; Huc, Ivan; Lehn, Jean-Marie; DeCian, Andre; Fischer, Jean
CORPORATE SOURCE: Laboratoire Chimie Supramoleculaire, Univ. Louis Pasteur, Strasbourg, F-67000, Fr.
SOURCE: European Journal of Organic Chemistry (1999), (11), 3089-3094
CODEN: EJOCFK; ISSN: 1434-193X
PUBLISHER: Wiley-VCH Verlag GmbH
DOCUMENT TYPE: Journal

h eb c g cg b cg eb

LANGUAGE: English

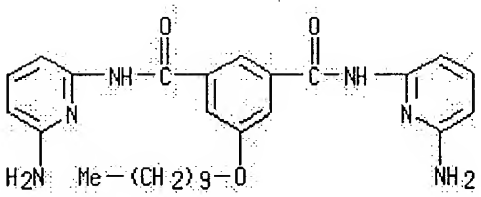
AB The selection of the receptor presenting the strongest affinity for a barbiturate substrate from a dynamic combinatorial library of constituents differing in structure and conformation/configuration is described. The gradual addn. of the barbiturate to an equilibrating mixt. of hydrazone isomers leads to the quant. shift towards a single species, 5,5-dibutylbarbiturate, which presents highest complementarity to the substrate and yields a supramol. entity with the bis(2-pyridinylhydrazone) of 5,5-dimethyl-1,3-cyclohexanedione.

IT **252903-90-5P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(induced-fit selection of barbiturate receptor from dynamic structural and conformational/configurational library)

RN 252903-90-5 HCAPLUS

CN 1,3-Benzenedicarboxamide, N,N'-bis(6-amino-2-pyridinyl)-5-(decyloxy)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 80 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | CITED References

ACCESSION NUMBER: 1999:684896 HCAPLUS

DOCUMENT NUMBER: 132:12145

TITLE: Hydrogen-bonding motifs in the crystals of secondary diamides with 2-amino-6-methyl- and 2,6-diaminopyridine subunits

AUTHOR(S): Mazik, Monika; Blaser, Dieter; Boese, Roland

CORPORATE SOURCE: Institut fur Organische Chemie der Universitat Essen, Essen, D-45117, Germany

SOURCE: Tetrahedron (1999), 55(44), 12771-12782
CODEN: TETRAB; ISSN: 0040-4020

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

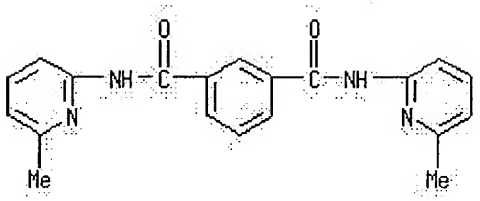
AB Hydrogen-bonding motifs in the crystal structures of N,N'-bis(6-methyl-pyridin-2-yl)isophthalamide, 1,3-bis[[(6-methyl-pyridin-2-yl)amino]carbonylmethyloxy]benzene, N,N'-bis(6-amino-pyridin-2-yl)isophthalamide and 1,3-bis[[(6-amino-pyridin-2-yl)amino]carbonylmethyloxy]benzene are reported. The hydrogen bond preferences were analyzed.

IT **251655-31-9P**

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(crystallog.; hydrogen-bonding motifs in the crystals of secondary diamides with 2-amino-6-methyl- and 2,6-diaminopyridine subunits)

RN 251655-31-9 HCAPLUS

CN 1,3-Benzenedicarboxamide, N,N'-bis(6-methyl-2-pyridinyl)-, hydrate (2:1) (9CI) (CA INDEX NAME)



1/2 H_2O

REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 81 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Cited References

ACCESSION NUMBER: 1999:643409 HCAPLUS
DOCUMENT NUMBER: 132:12561
TITLE: Glucopyranoside Recognition by Polypyridine-Macrocyclic Receptors Possessing a Wide Cavity with a Flexible Linkage
AUTHOR(S): Inouye, Masahiko; Chiba, Junya; Nakazumi, Hiroyuki
CORPORATE SOURCE: PRESTO Japan Science and Technology Corporation (JST) Department of Applied Materials Science, Osaka Prefecture University, Sakai Osaka, 599-8531, Japan
SOURCE: Journal of Organic Chemistry (1999), 64(22), 8170-8176 CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB New polypyridine-macrocyclic receptors for glucopyranosides were designed and synthesized. The artificial receptors possess a terpyridine skeleton as a hydrogen-bonding site and a flexible polyoxyethylene chain as a bridge for the macrocyclic structure, in which the cavity of the receptors is large enough to incorporate pyranosides. The receptors showed high affinities for n-octyl β-(D)-glucopyranoside, and selective binding of the receptors was obsd. between epimeric pyranosides. The results obtained in this paper demonstrated versatility of the terpyridine skeleton as a hydrogen-bonding site for saccharides.

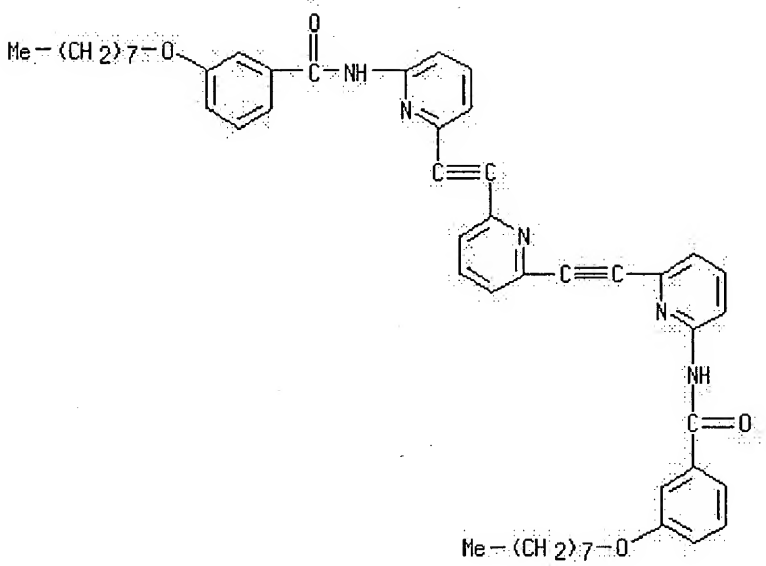
IT **251640-44-5P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (prepn. and mol. structure of polypyridine-macrocyclic receptors contg. terpyridine skeleton as a hydrogen-bonding site for glucopyranosides)

RN 251640-44-5 HCAPLUS
CN β-D-Ribofuranoside, methyl, compd. with N,N'-[2,6-pyridinediylbis(2,1-ethynediyl-6,2-pyridinediyl)]bis[3-(octyloxy)benzamide] (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 251640-40-1
CMF C49 H53 N5 O4

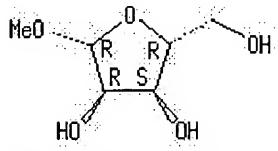
h eb c g cg b cg eb



CM 2

CRN 7473-45-2
CMF C6 H12 O5

Absolute stereochemistry.



REFERENCE COUNT: 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 82 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Other Sources | References

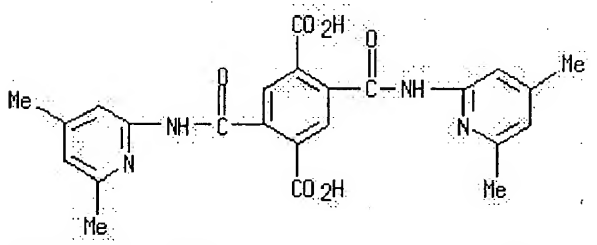
ACCESSION NUMBER: 1999:571294 HCAPLUS
DOCUMENT NUMBER: 131:295122
TITLE: NMR-based discovery of phosphotyrosine mimetics that bind to the Lck SH2 domain
AUTHOR(S): Hajduk, Philip J.; Zhou, Ming-Ming; Fesik, Stephen W.
CORPORATE SOURCE: Abbott Laboratories, Abbott Park, IL, 60064, USA
SOURCE: Bioorganic & Medicinal Chemistry Letters (1999), 9(16), 2403-2406
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Using an NMR-based screen, a series of novel phosphotyrosine mimetics were discovered that bind to the SH2 domain of Lck. These compds. may serve as useful leads for the design of nonpeptide inhibitors of SH2 domains with improved bioavailability and metabolic stability compared to the natural ligands that contain phosphotyrosine.

IT **247089-00-5**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(NMR-based discovery of phosphotyrosine mimetics that bind to Lck SH2

h eb c g cg b cg eb

domain)
RN 247089-00-5 HCAPLUS
CN 1,4-Benzenedicarboxylic acid, 2,5-bis[[(4,6-dimethyl-2-pyridinyl)amino]carbonyl]- (9CI) (CA INDEX NAME)

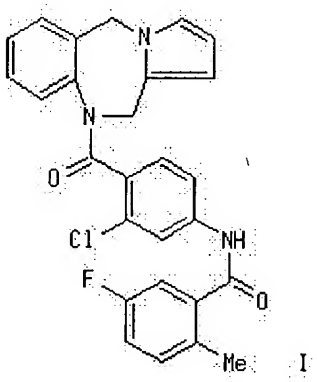


REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 83 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 1999:429264 HCAPLUS
DOCUMENT NUMBER: 131:184927
TITLE: 5-Fluoro-2-methyl-N-[5-(5H-pyrrolo[2,1-c][1,4]benzodiazepin-10(11H)-ylcarbonyl)-2-pyridinyl]benzamide (CL-385004) and analogs as orally active arginine vasopressin receptor antagonists
AUTHOR(S): Aranapakam, Venkatesan; Albright, J. Donald; Grosu, George T.; Delos Santos, Efren G.; Chan, Peter S.; Coupet, Joseph; Ru, Xun; Saunders, Trina; Mazandarani, H.
CORPORATE SOURCE: Wyeth-Ayerst Research, Pearl River, NY, 10965, USA
SOURCE: Bioorganic & Medicinal Chemistry Letters (1999), 9(13), 1737-1740
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

AB Synthesis and structure-activity relationships of orally active arginine vasopressin (AVP) receptor antagonists are discussed. Potent and orally active AVP receptor antagonists are produced when the central benzene ring of VPA-985 (I) is replaced with a 3-pyridinyl unit.

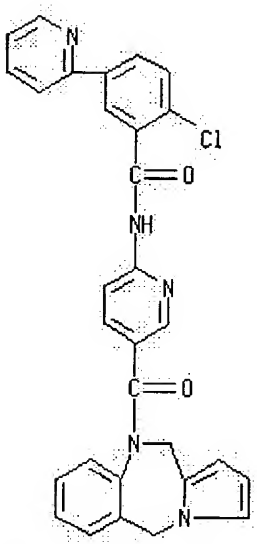
IT **239450-11-4P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological

h eb c g cg b cg eb

study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(prepn. as orally active arginine vasopressin receptor antagonist)

RN 239450-11-4 HCAPLUS

CN Benzamide, 2-chloro-5-(2-pyridinyl)-N-[5-(5H-pyrrolo[2,1-c][1,4]benzodiazepin-10(11H)-ylcarbonyl)-2-pyridinyl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 84 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

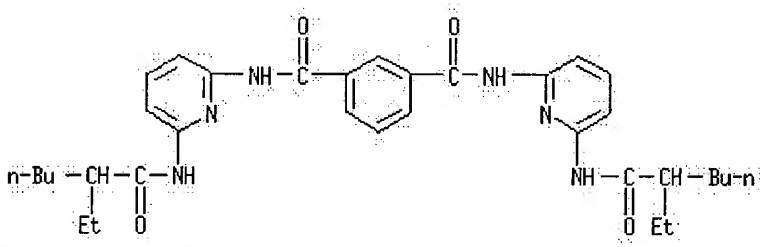
Full Text | Citing References

ACCESSION NUMBER: 1999:245257 HCAPLUS
DOCUMENT NUMBER: 131:53493
TITLE: Artificial Receptor-Facilitated Solid-Phase Microextraction of Barbiturates
AUTHOR(S): Li, Shu; Sun, Lifang; Chung, Yongsoon; Weber, Stephen G.
CORPORATE SOURCE: Department of Chemistry, University of Pittsburgh, Pittsburgh, PA, 15260, USA
SOURCE: Analytical Chemistry (1999), 71(11), 2146-2151
CODEN: ANCHAM; ISSN: 0003-2700
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A receptor for barbiturates, N,N'-Bis-[6-(2-ethylhexanoylamino)-pyridin-2-yl]-isophthalamide, was designed to dissolve in plasticizers of poly(vinyl chloride) (PVC). Microextns. using receptor-doped films of PVC were carried out as a function of receptor concn. The effect of the concn. of the receptor on extn. yield is considerable for barbiturates that have significant binding to the receptor but negligible for very similar mols. that do not bind to the receptor strongly. Thus, it is the receptor's ability in mol. recognition, not its generic ability as an H-bonding cosolvent, that is important. On the other hand, NMR data show that the receptor self-assocs. A simple, approx. anal. is given to ext. the amt. of active receptor from the data. Receptor-enhanced extns. of barbiturates from urine are compared to extns. using a phosphate ester as solvent.

h eb c g cg b cg eb

IT **228271-35-0P**
RL: ARG (Analytical reagent use); BUU (Biological use, unclassified); SPN (Synthetic preparation); ANST (Analytical study); BIOL (Biological study); PREP (Preparation); USES (Uses)
(artificial receptor-facilitated solid-phase microextn. of barbiturates)
RN 228271-35-0 HCAPLUS
CN 1,3-Benzenedicarboxamide, N,N'-bis[6-[(2-ethyl-1-oxohexyl)amino]-2-pyridinyl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 85 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN
Full Text | CITING References

ACCESSION NUMBER: 1999:241334 HCAPLUS
DOCUMENT NUMBER: 130:329555
TITLE: Hydrogen bonding association of a ruthenium(II) bipyridine barbituric acid guest to complementary 2,6-diamino-pyridine amide hosts: guidelines for designing high binding hydrogen bonding cavities in both high-and low-polarity solvents
AUTHOR(S): Salameh, A. S.; Ghaddar, T.; Isied, Stephan S.
CORPORATE SOURCE: American University of Beirut, Beirut, Lebanon
SOURCE: Journal of Physical Organic Chemistry (1999), 12(3), 247-254
CODEN: JPOCEE; ISSN: 0894-3230
PUBLISHER: John Wiley & Sons Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The binding between a Ru polypyridine guest RuG2, (Ru = 4,4'-di-tert-butyl-bpy)2Ru (bpy = 2,2'-bipyridine) and G2 = 5-[4-(4'-methyl)-2,2'-bipyridyl]methyl-2,4,6-(1H,3H,5H)-pyrimidinetrione, and host acyl derivs. of 3,5-bis[(6-aminopyrid-2-yl) amino]carbonylpyridine (R/H = Pr/H, phenyl/H, CF3/H, t-Bu/H, -(CH2)3-CO2-H) and 3,5-bis[(6-amino-4-isopropoxypyrid-2-yl)amino]carbonylpyridine diacetyl deriv. (R/X = CH3/i-OPr) were studied by fluorescence and NMR titrns. The RuG2 (which exists in the enolate form in the presence of the hosts) forms a no. of H-bonds involving the amide groups of the hosts and the carbonyl groups of the G2 for all the hosts studied. Specific 1:1 assocn. between RuG2 and all the complementary hosts was obsd. with binding consts., Ka (1 mol-1), for R/H in CH2Cl2 of 3 105 ± (t-Bu/H), 5 106 ± (Ph/H), 3 107 ± (Pr/H), 9 107 ± (CF3/H) and >108 [-(CH2)3CO2H] and for R/X of 4 108 ± (Me/i-OPr). Similar, but weaker, binding was also obsd. in solvents of higher donor no. such as d6-acetone, d3-MeCN and d6-DMSO with R/X = Me/i-OPr host showing the highest binding const. in CH2Cl2, d6-acetone and d6-DMSO. Differences in the binding consts. of the Ru guest RuG2 to these hosts are analyzed in terms of the steric, electronic and solvation changes in the structure of the host amide substituents and

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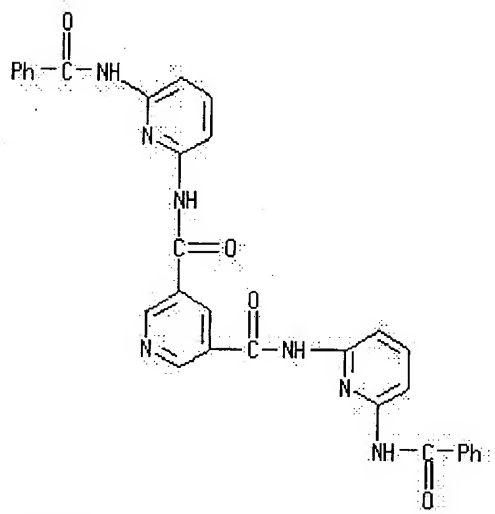
the polarity of the solvents used.

IT **223708-96-1P**

RL: PEP (Physical, engineering or chemical process); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)
(prepn. and assocn. consts. and hydrogen bonding with ruthenium bipyridylmethylpyrimidinetrione complex)

RN 223708-96-1 HCAPLUS

CN 3,5-Pyridinedicarboxamide, N,N'-bis[6-(benzoylamino)-2-pyridinyl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 86 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 1999:186121 HCAPLUS
DOCUMENT NUMBER: 130:329456
TITLE: Design of New Organic Gelators Stabilized by a Host-Guest Interaction
AUTHOR(S): Inoue, Kazuhiko; Ono, Yoshiyuki; Kanekiyo, Yasumasa; Ishi-i, Tsutomu; Yoshihara, Kanami; Shinkai, Seiji
CORPORATE SOURCE: Chemotransfiguration Project, Japan Science and Technology Corporation (JST), Kurume Fukuoka, 839-0861, Japan
SOURCE: Journal of Organic Chemistry (1999), 64(8), 2933-2937
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The present paper demonstrated that new org. gelators can be designed by an appropriate combination of H-bonding hosts and guests. The authors synthesized 2 host compds. which possess a 2,6-(dimethylamino)pyridine moiety; 1,3-Bis[[(6-cholesteryloxyformamido-2-pyridyl)amino]carbonyl]propane (HostI) and 1,3-Bis[[(6-cholesteryloxyformamido-2-pyridyl)amino]carbonyl]benzene (HostII). Two different gelation mechanisms are identified: (i) the HostI/guest system increases the free NH group and forms the gel by the intermol. H-bonding interaction (ii) the HostII/guest system decreases the free NH group and forms the complementary host-guest complex useful for the intermol. stacking.

IT **223749-92-6P**

h eb c g cg b cg eb

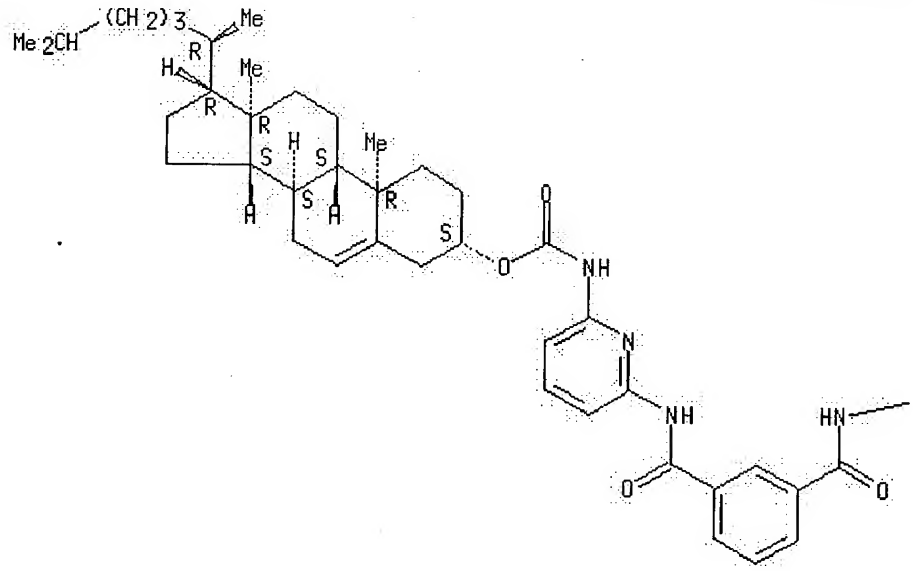
RL: PEP (Physical, engineering or chemical process); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)
(synthesis of host compd. contg. (dimethylamino)pyridine moiety to prep. new org. gelators stabilized by host-guest interaction)

RN 223749-92-6 HCAPLUS

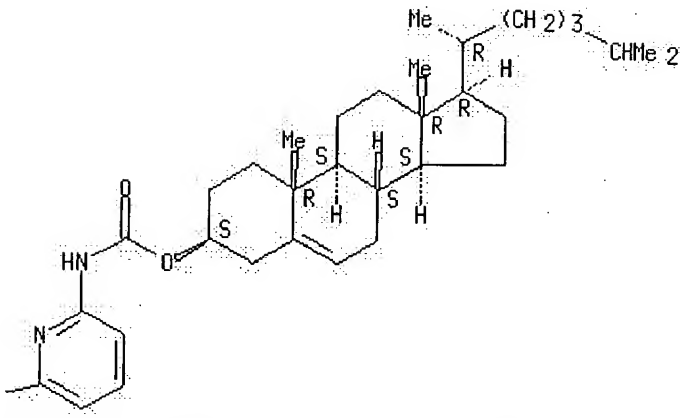
CN Cholest-5-en-3-ol (3β)-, [1,3-phenylenebis(carbonylimino-6,2-pyridinediyl)]bis[carbamate] (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



REFERENCE COUNT: 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

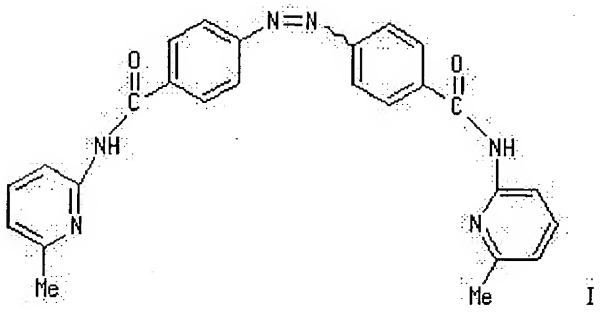
L12 ANSWER 87 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 1999:126086 HCAPLUS
DOCUMENT NUMBER: 130:281735
TITLE: Molecular recognition: hydrogen bonding induced configurational locking of a new photoresponsive receptor by dicarboxylic acids

h eb c g cg b cg eb

AUTHOR(S): Goswami, Shyamaprosad; Ghosh, Kumaresh; Halder, Mintu
CORPORATE SOURCE: Department of Chemistry, Bengal Engineering College, Deemed University, Howrah, 711 103, India
SOURCE: Tetrahedron Letters (1999), 40(9), 1735-1738
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



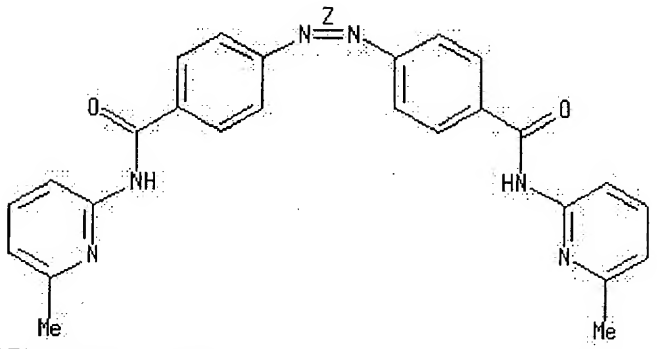
I

AB A new photoresponsive system (I) has been synthesized and recognition by the cavity of the cis-isomer of I of dicarboxylic acids of various chain lengths has been studied on irradn. at 310 nm. The cavity of the cis form is found to be selective for adipic acid.

IT 222529-63-7P
RL: PEP (Physical, engineering or chemical process); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); PROC (Process); RACT (Reactant or reagent)
(prepn. of functionalized azo compd. as azo receptor for dicarboxylic acids)

RN 222529-63-7 HCAPLUS
CN Benzamide, 4,4'-(1Z)-azobis[N-(6-methyl-2-pyridinyl)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 88 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | String References

ACCESSION NUMBER: 1999:83191 HCAPLUS
DOCUMENT NUMBER: 130:222967
TITLE: Influence of remote intramolecular hydrogen bonds on

h eb c g cg b cg eb

the thermodynamics of molecular recognition of cis-1,3,5-cyclohexanetricarboxylic acid

AUTHOR(S): Ballester, Pablo; Costa, Antoni; Deya, Pere M.; Vega, Manuel; Morey, Jeroni; Deslongchamps, Ghislain

CORPORATE SOURCE: Department de Quimica. Universitat de les Illes Balears, Palma de Mallorca, 07071, Spain

SOURCE: Tetrahedron Letters (1999), 40(1), 171-174
CODEN: TELEAY; ISSN: 0040-4039

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

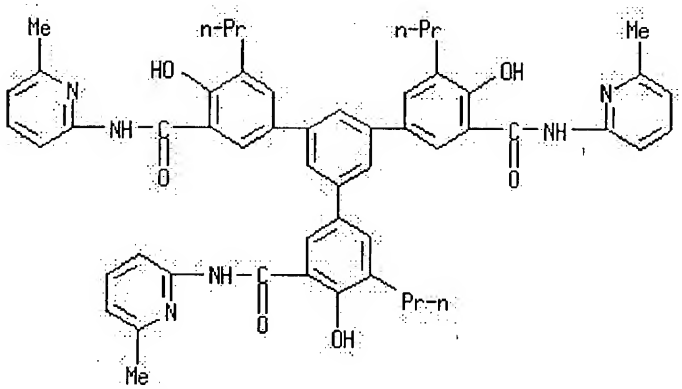
LANGUAGE: English

AB Variable temp. binding studies and isothermal titrn. microcalorimetry were used to probe the thermodn. of mol. recognition of cis-1,3,5-cyclohexanetricarboxylic acid by tripodal hosts. Remote intramol. hydrogen bonds, used to restrict conformationally one of the hosts, exhibit a strong influence on the thermodn. functions for the binding process ΔH and ΔS, with little effect on ΔG. This suggests that the conformational lock imposed by the intramol. hydrogen bonds organizes the receptor in a conformation that is not optimal for the binding of the triacid.

IT **157460-60-1**
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)
(effect of remote intramol. hydrogen bonds on the thermodn. of mol. recognition of cis-1,3,5-cyclohexanetricarboxylic acid)

RN 157460-60-1 HCAPLUS

CN [1,1':3',1''-Terphenyl]-3,3''-dicarboxamide, 4,4''-dihydroxy-5'-[4-hydroxy-3-[[(6-methyl-2-pyridinyl)amino]carbonyl]-5-propylphenyl]-N,N'-bis(6-methyl-2-pyridinyl)-5,5''-dipropyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 89 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 1999:42574 HCAPLUS

DOCUMENT NUMBER: 130:95485

TITLE: Preparation of bisamides pyridinediamines as antithrombotic agents

INVENTOR(S): Beight, Douglas Wade; Craft, Trelia Joyce; Franciskovich, Jeffry Bernard; Goodson, Theodore, Jr.; Hall, Steven Edward; Herron, David Kent; Klimkowski, Valentine Joseph; Kyle, Jeffrey Alan; Masters, John Joseph; Mendel, David; Milot, Guy; Sawyer, Jason Scott; Shuman, Robert Theodore; Smith, Gerald Floyd;

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Tebbe, Anne Louise; Tinsley, Jennifer Marie; Weir, Leonard Crayton; Wikel, James Howard; Wiley, Michael Robert; Yee, Ying Kwong
PATENT ASSIGNEE(S): Eli Lilly and Company, USA
SOURCE: PCT Int. Appl., 80 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9900126	A1	19990107	WO 1998-US13384	19980626
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
AU 9882693	A1	19990119	AU 1998-82693	19980626
EP 999834	A1	20000517	EP 1998-932911	19980626
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, FI				
JP 2002506462	T2	20020226	JP 1999-505809	19980626
US 6313151	B1	20011106	US 2000-445973	20000331
US 2002049234	A1	20020425	US 2001-967203	20010928
US 6586459	B2	20030701		
US 2002072531	A1	20020613	US 2001-967054	20010928
US 6583173	B2	20030624		

PRIORITY APPLN. INFO.: US 1997-50881P P 19970626
WO 1998-US13384 W 19980626
US 2000-445973 A3 20000331

OTHER SOURCE(S): MARPAT 130:95485
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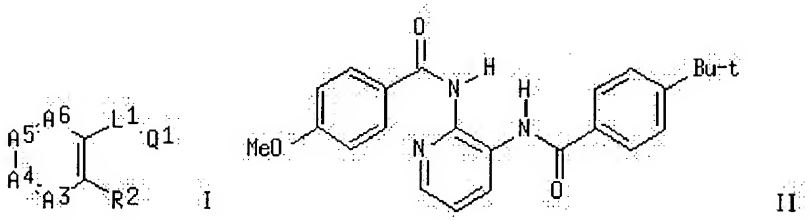

AB The title compds. [I; A3-A6 together with the two carbons to which they are attached = heterocyclic ring (in which (a) one of A3-A6 = N, and each of the others = CR3, CR4, CR5 or CR6, resp.; (b) two adjacent residues of A3-A6 together form S; (c) two non-adjacent residues of A3-A6 = N; (d) A3 and A4 together form a fused benzene ring, and A5 and A6 together form NH; each of R3-R6 = H, or one or two of R3-R6 = Cl, Br, Me and the others = H); L1 = NHCO, CONH; Q1 = (un)substituted Ph, 2-furanyl, 2-thienyl, etc.; R2 = 4-MeOC6H4CONH, 4-tBuC6H4CONH, etc.], useful as inhibitors of factor Xa, were prepd. and formulated. Thus, 3-step synthesis of II, starting with N3-(tert-butoxycarbonyl)-N2-(4-methoxybenzoyl)-2,3-pyridinediamine, was described. In general, compds. I exhibit a Kass of 0.1-0.5x106 L/Mol or much greater for human factor Xa.

IT **219493-51-3P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological

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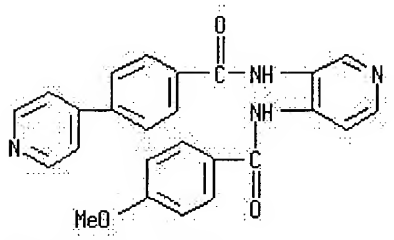
study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of bisamides pyridinediamines as antithrombotic agents)

RN 219493-51-3 HCAPLUS

CN Benzamide, N-[4-[(4-methoxybenzoyl)amino]-3-pyridinyl]-4-(4-pyridinyl)-(9CI) (CA INDEX NAME)



REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 90 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 1999:17723 HCAPLUS
DOCUMENT NUMBER: 130:217600
TITLE: Three-Dimensional Quantitative Structure-Activity Relationship Study on Cyclic Urea Derivatives as HIV-1 Protease Inhibitors: Application of Comparative Molecular Field Analysis
AUTHOR(S): Debnath, Asim Kumar
CORPORATE SOURCE: Biochemical Virology Laboratory, Lindsley F. Kimball Research Institute of The New York Blood Center, New York, NY, 10021, USA
SOURCE: Journal of Medicinal Chemistry (1999), 42(2), 249-259
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Three-dimensional quant. structure-activity relationship (3D-QSAR) models have been developed using comparative mol. field anal. (CoMFA) on a large data set (118 compds.) of diverse cyclic urea derivs. as protease inhibitors against the human immunodeficiency virus type 1 (HIV-1). X-ray crystal structures of HIV-1 protease bound with this class of inhibitors were used to derive the most probable bioactive conformations of the inhibitors. The enzyme active site was used as a constraint to limit the no. of possible conformations that are sterically accessible. The test sets have been created keeping in mind structural diversity as well as the uniform simple statistical criteria (mean, std. deviation, high and low values) of the protease inhibitory activities of the mols. compared to the training sets. Multiple predictive models have been developed with the training sets (93 compds. in each set) and validated with the corresponding test sets (25 compds. in each set). All the models yielded high predictive correlation coeffs. (q2 from 0.699 to 0.727), substantially high fitted correlation coeffs. (r2 from 0.965 to 0.973), and reasonably low std. errors of ests. (S from 0.239 to 0.265). The steric and electrostatic effects have approx. equal contributions, 45% and 55% (approx.), resp., toward explaining protease inhibitory activities. This anal. yielded models with significant information on steric and electrostatic interactions clearly discerned by the resp. coeff. contour plots when overlapped on the X-ray structure of the HIV-1 protease. The HINT CoMFA study revealed significant contribution of hydrophobicity

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toward protease inhibitory activity. The 3D visualization technique utilizing these contour plots as well as the receptor site geometry may significantly improve our understanding of the inhibitor-protease (HIV-1) interactions and help in designing compds. with improved activity.

IT **183854-97-9**

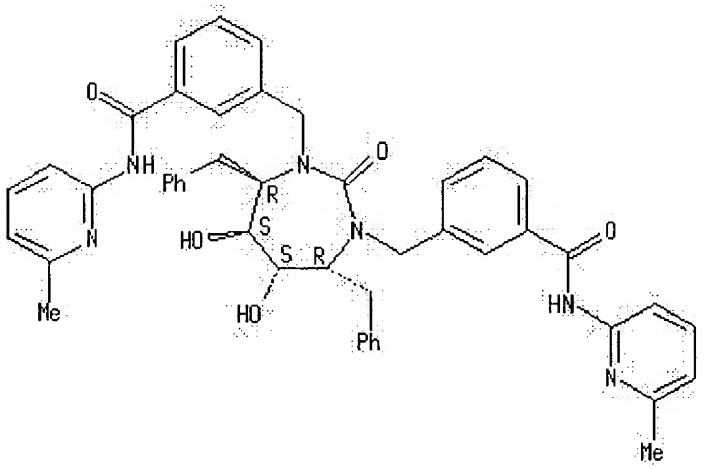
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(QSAR study on cyclic urea derivs. as HIV-1 protease inhibitors: application of comparative mol. field anal.)

RN 183854-97-9 HCAPLUS

CN Benzamide, 3,3'-[[(4R,5S,6S,7R)-tetrahydro-5,6-dihydroxy-2-oxo-4,7-bis(phenylmethyl)-1H-1,3-diazepine-1,3(2H)-diyl]bis(methylene)]bis[N-(6-methyl-2-pyridinyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 57 THERE ARE 57 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 91 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 1998:782620 HCAPLUS
DOCUMENT NUMBER: 130:125047
TITLE: Stereospecific Synthesis, Structure-Activity Relationship, and Oral Bioavailability of Tetrahydropyrimidin-2-one HIV Protease Inhibitors
AUTHOR(S): De Lucca, George V.; Liang, Jing; De Lucca, Indawati
CORPORATE SOURCE: DuPont Pharmaceuticals Company, Wilmington, DE, 19880-0500, USA
SOURCE: Journal of Medicinal Chemistry (1999), 42(1), 135-152
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The use of tetrahydropyrimidinones as an alternate scaffold for designing HIVPR inhibitors has advantages, over the previously disclosed hexahydro-1,3-diazepin-2-ones, of being more unsym., less cryst., more sol., and more lipophilic. They show a better translation of Ki to IC90 for the more polar P2 groups that in general give the more potent enzyme inhibitors. Structure-activity relationship (SAR) studies of the tetrahydropyrimidinones showed that the phenylethyl P1' substituent, the hydroxyl group, and the urea carbonyl are all crit. for good activity.

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However, there was significant flexibility in the possible P2/P2' substituents that could be used. Many analogs that contained identical or different P2/P2' substituents, or only one P2 substituent, had excellent enzyme potency and several had excellent antiviral potency. Several of these compds. were examd. for oral bioavailability in the rat or the dog at 10 mg/kg. However, the oral bioavailability of the tetrahydropyrimidinones was, in general, less than for the corresponding hexahydro-1,3-diazepin-2-ones. Unfortunately, when all factors are considered, including potency, protein binding, soly., bioavailability, and resistance profile, the tetrahydropyrimidinones did not offer any advantage over the previously disclosed hexahydro-1,3-diazepin-2-ones series.

IT **219941-25-0P**

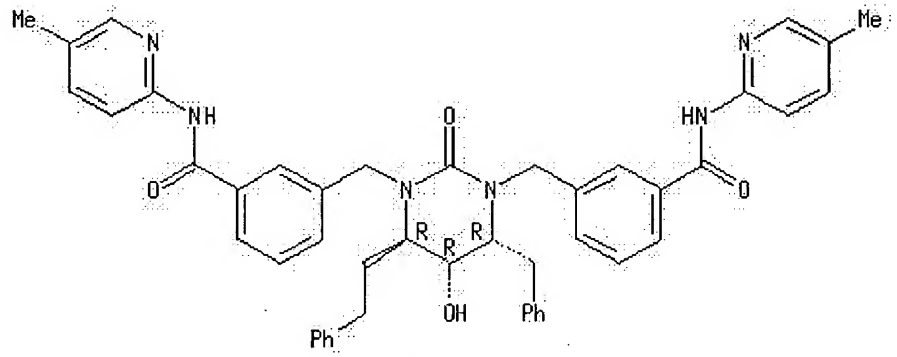
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(prepn., structure-activity relationship, and oral bioavailability of tetrahydropyrimidinone HIV protease inhibitors)

RN 219941-25-0 HCAPLUS

CN Benzamide, 3,3'-[[(4R,5R,6R)-dihydro-5-hydroxy-2-oxo-4-(2-phenylethyl)-6-(phenylmethyl)-1,3(2H,4H)-pyrimidinediyl]bis(methylene)]bis[N-(5-methyl-2-pyridinyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 92 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 1998:447028 HCAPLUS
DOCUMENT NUMBER: 129:221600
TITLE: Molecular Recognition on Functionalized Self-Assembled Monolayers of Alkanethiols on Gold
AUTHOR(S): Motesharei, Kianoush; Myles, David C.
CORPORATE SOURCE: Department of Chemistry Biochemistry, University of California, Los Angeles, CA, 90095-1569, USA
SOURCE: Journal of the American Chemical Society (1998), 120(29), 7328-7336
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A system for probing mol. recognition events at org. interfaces using fluorescent receptors is described. Receptors formed from the bis(2,6-diaminopyridine) amide of isophthalic acid are incorporated in mixed self-assembled monolayers (SAMs) of alkanethiols on gold and shown

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to interact with barbituric acid derivs. from soln. Individual parameters that affect the ability of receptors on surfaces to recognize ligands from soln. along with varieties of solvents for ligand solns. were examd.

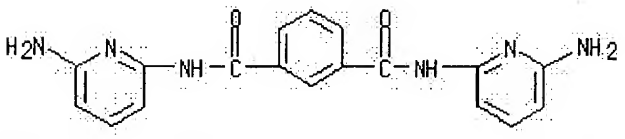
IT **112817-57-9P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(interaction of barbituric acid derivs. with mixed monolayers of alkanethiols and bis(2,6-diaminopyridine) amide of isophthalic acid-functionalized decanethiol on thin gold films)

RN 112817-57-9 HCAPLUS

CN 1,3-Benzenedicarboxamide, N,N'-bis(6-amino-2-pyridinyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 77 THERE ARE 77 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 93 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 1998:423341 HCAPLUS

DOCUMENT NUMBER: 129:189216

TITLE: Synthetic analogs of netropsin and distamycin - synthesis of a new pyridine and carbocyclic analogs of the pyrrolecarboxamide antitumor antibiotics

AUTHOR(S): Bartulewicz, Danuta; Bielawski, Krzysztof; Markowska, Agnieszka; Zwierz, Krzysztof; Puckowska, Anna; Rozanski, Andrzej

CORPORATE SOURCE: Department of Organic Chemistry, Medical Academy, Bialystok, 15-230, Pol.

SOURCE: Acta Biochimica Polonica (1998), 45(1), 41-57
CODEN: ABPLAF; ISSN: 0001-527X

PUBLISHER: Polish Biochemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

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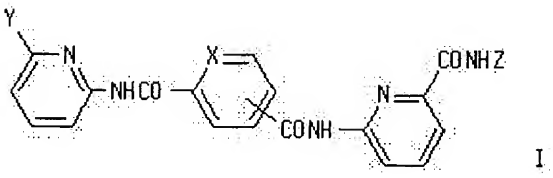

I

AB A new series of pyridine-contg. analogs of distamycin A (I; X = N, C; Y = H, substituted pyridyl, CONH(CH2)3NMe2; Z = (CH2)nNMe2, substituted pyridyl; n = 2, 3) and netropsin was investigated by the mol. mechanics technique and mol. modeling. Some of I were prepd. as potential carriers of alkylating elements and carriers to place into the minor groove of DNA chem. groups capable of modifying DNA.

IT **189000-55-3P**

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); MSC (Miscellaneous); PNU (Preparation, unclassified); THU (Therapeutic use); BIOL (Biological study); PREP

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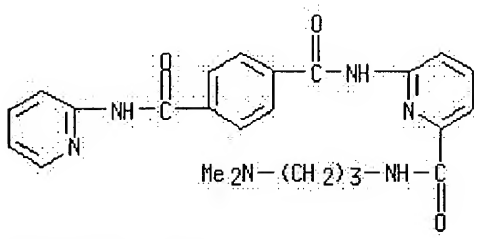
(Preparation); USES (Uses)
(synthetic analogs of netropsin and distamycin - synthesis of a new pyridine and carbocyclic analogs of the pyrrolecarboxamide antitumor antibiotics)

RN 189000-55-3 HCAPLUS

CN 1,4-Benzenedicarboxamide, N-[6-[[[3-(dimethylamino)propyl]amino]carbonyl]-2-pyridinyl]-N'-2-pyridinyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 41 THERE ARE 41 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 94 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 1998:421320 HCAPLUS
DOCUMENT NUMBER: 129:89888
TITLE: Comparative Molecular Field Analysis (CoMFA) of a Series of Symmetrical Bis-Benzamide Cyclic Urea Derivatives as HIV-1 Protease Inhibitors
AUTHOR(S): Debnath, Asim Kumar
CORPORATE SOURCE: Biochemical Virology Laboratory Lindsley F. Kimball Research Institute, New York Blood Center, New York, NY, 10021, USA
SOURCE: Journal of Chemical Information and Computer Sciences (1998), 38(4), 761-767
CODEN: JCISD8; ISSN: 0095-2338
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A 3D-QSAR study using CoMFA methodol. was conducted on a series of 29 sym. bis-benzamide cyclic urea derivs. having anti-HIV-1-protease activities. Active site minimization of the ligands was used to exclude conformations which are not sterically accessible within the active site. A significant cross-validated correlation coeff. q2 (0.724) was obtained indicating the predictive potential of the model for untested compds. of this class. A significant non-cross-validated correlation coeff. (r2) of 0.971 with a low std. error est. (S) of 0.119 was obtained indicating that the model reliably predicted the anti-protease activities of poorly to highly active compds. The model was used to predict the anti-protease activities of 8 test-set compds., and the predicted values were in good agreement with the exptl. values. The CoMFA coeff. contour plots identified several key features which explain the wide range of activities. The already reported 2D-QSAR along with the CoMFA model presented here may help in designing effective HIV-1 protease inhibitors.

IT **183854-97-9**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)
(CoMFA of bisbenzamide cyclic ureas as HIV-1 protease inhibitors)

RN 183854-97-9 HCAPLUS

CN Benzamide, 3,3'-[[(4R,5S,6S,7R)-tetrahydro-5,6-dihydroxy-2-oxo-4,7-bis(phenylmethyl)-1H-1,3-diazepine-1,3(2H)-diyl]bis(methylene)]bis[N-(6-

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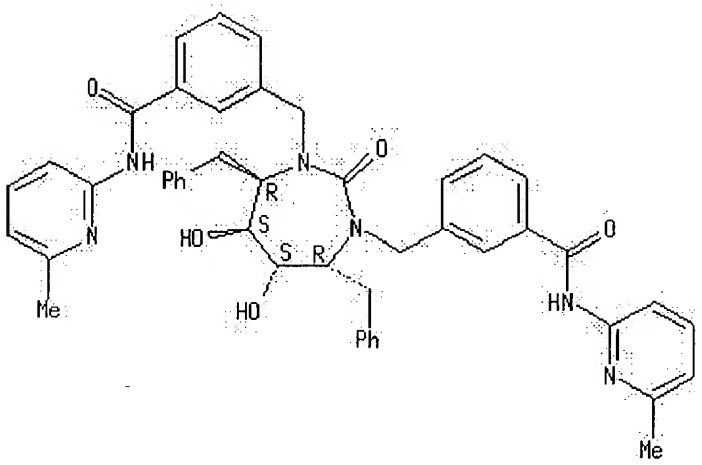
methyl-2-pyridinyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 95 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 1998:372652 HCAPLUS
DOCUMENT NUMBER: 129:54368
TITLE: Preparation of 9-heterocyclylalkyl-9-fluorenecarboxamides and analogs as microsomal triglyceride transfer protein inhibitors
INVENTOR(S): Biller, Scott A.; Dickson, John K.; Lawrence, R. Michael; Magnin, David R.; Poss, Michael A.; Robl, Jeffrey A.; Slusarchyk, William A.; Sulsky, Richard B.; Tino, Joseph A.
PATENT ASSIGNEE(S): USA
SOURCE: U.S., 240 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5760246	A	19980602	US 1996-767923	19961217
US 6472414	B1	20021029	US 1999-313883	19990518

PRIORITY APPLN. INFO.: US 1996-767923 A1 19961217
US 1997-802705 B1 19970219
OTHER SOURCE(S): MARPAT 129:54368
GI

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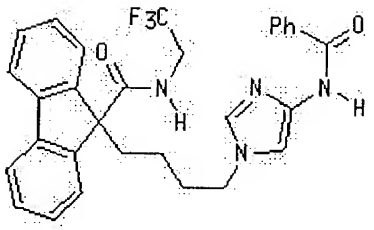


I

AB Title compds., e.g., R1Z1BCOAZ2R2 [A = bond, O, (alkyl)imino; B = e.g., C(ZR)2 in which RR = bond, O, NH, alk(en)ylene, etc., and Z = (un)substituted 1,2-phenylene; R1 = H, alk(en)yl, (hetero)aryl, etc.; R1 = groups cited for R1, haloalkyl, etc.; Z1 = (oxo- or aza)(oxo)alk(en)ylene, etc.; Z2 = bond, groups cited forZ1, etc.] were prepd. as microsomal triglyceride transfer protein inhibitors (no data). Thus, 9-fluorenecarboxylic acid was alkylated by Br(CH2)4Br and the CF3CH2NH2-amidated product arylated by 4-nitroimidazole to give, after redn. and N-acylation, title compd I.

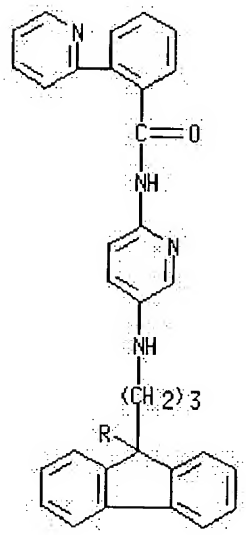
IT **194214-02-3P**

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of 9-heterocyclylalkyl-9-fluorenecarboxamides and analogs as microsomal triglyceride transfer protein inhibitors)

RN 194214-02-3 HCAPLUS

CN 9H-Fluorene-9-carboxamide, 9-[3-[[6-[[2-(2-pyridinyl)benzoyl]amino]-3-pyridinyl]amino]propyl]-N-(2,2,2-trifluoroethyl)-, dihydrochloride (9CI) (CA INDEX NAME)

PAGE 1-A



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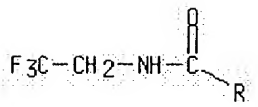
PAGE 2-A



2 HCl

REFERENCE COUNT: 44 THERE ARE 44 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 96 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 1998:331766 HCAPLUS
DOCUMENT NUMBER: 129:89939
TITLE: Resistance to HIV Protease Inhibitors: A Comparison of Enzyme Inhibition and Antiviral Potency
AUTHOR(S): Klabe, Ronald M.; Bacheler, Lee T.; Ala, Paul J.; Erickson-Viitanen, Susan; Meek, James L.
CORPORATE SOURCE: Departments of Virology and of Physical and Chemical Sciences, DuPont Merck Pharmaceutical Company, Wilmington, DE, 19880-0336, USA
SOURCE: Biochemistry (1998), 37(24), 8735-8742
CODEN: BICHAW; ISSN: 0006-2960
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Resistance of HIV-1 to protease inhibitors has been assocd. with changes at residues Val82 and Ile84 of HIV-1 protease (HIV PR). Using both an enzyme assay with a peptide substrate and a cell-based infectivity assay, we examd. the correlation between the inhibition consts. for enzyme activity (Ki values) and viral replication (IC90 values) for 5 active site mutants and 19 protease inhibitors. Four of the five mutations studied (V82F, V82A, I84V, and V82F/I84V) had been identified as conferring resistance during in vitro selection using a protease inhibitor. The mutant protease genes were expressed in Escherichia coli for prepn. of enzyme, and inserted into the HXB2 strain of HIV for test of antiviral activity. The inhibitors included saquinavir, indinavir, nelfinavir, 141W94, ritonavir (all in clin. use), and 14 cyclic ureas with a const. core structure and varying P2, P2' and P3, P3' groups. The single mutations V82F and I84V caused changes with various inhibitors ranging from 0.3- to 86-fold in Ki and from 0.1- to 11-fold in IC90. Much larger changes compared to wild type were obsd. for the double mutation V82F/I84V both for Ki (10-2000-fold) and for IC90 (0.7-377-fold). However, there were low correlations (r2 = 0.017-0.53) between the mutant/wild-type ratio of Ki values (enzyme resistance) and the mutant/wild-type ratio of viral IC90 values (antiviral resistance) for each of the HIV proteases and the viruses contg. the identical enzyme. Assessing enzyme resistance by "vitality values", which adjust the Ki values with the catalytic efficiencies (kcat/Km), caused no significant improvement in the correlation with antiviral resistance. Therefore, our data suggest that measurements of enzyme inhibition with mutant proteases may be poorly predictive of the antiviral effect in resistant viruses even when mutations are restricted to the protease gene.

IT **183854-97-9**

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(resistance to HIV protease inhibitors and comparison of enzyme

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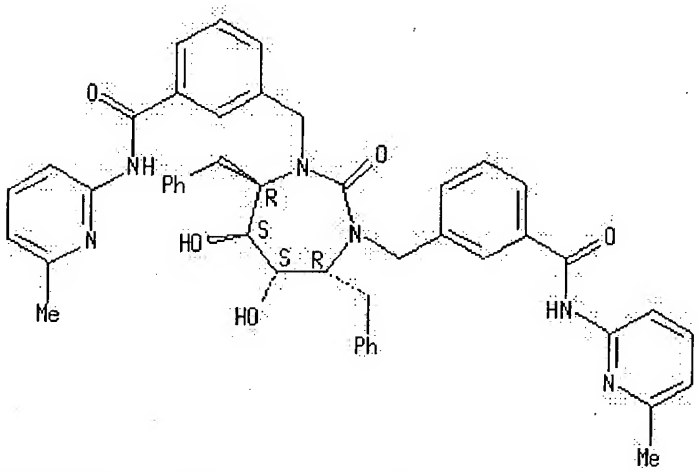
inhibition and antiviral potency using mutant proteases)
RN 183854-97-9 HCAPLUS
CN Benzamide, 3,3'-[[(4R,5S,6S,7R)-tetrahydro-5,6-dihydroxy-2-oxo-4,7-bis(phenylmethyl)-1H-1,3-diazepine-1,3(2H)-diyl]bis(methylene)]bis[N-(6-methyl-2-pyridinyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 97 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 1998:324820 HCAPLUS
DOCUMENT NUMBER: 129:16148
TITLE: Preparation of tricyclic benzodiazepines as vasopressin antagonists
INVENTOR(S): Albright, Jay Donald; Venkatesan, Aranapakam M.; Dusza, John P.; Sum, Fuk-wah
PATENT ASSIGNEE(S): American Cyanamid Co., USA
SOURCE: U.S., 119 pp., Cont.-in-part of U.S. 5,536,718.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 4
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5753648	A	19980519	US 1996-672150	19960627
US 5536718	A	19960716	US 1995-373132	19950117
CA 2258885	AA	19971231	CA 1997-2258885	19970620
WO 9749707	A1	19971231	WO 1997-US10736	19970620
W: AL, AU, BA, BB, BG, BR, CA, CN, CU, CZ, EE, GE, GH, HU, IL, IS, JP, KP, KR, LC, LK, LR, LT, LV, MG, MK, MN, MX, NO, NZ, PL, RO, RU, SG, SI, SK, SL, TR, TT, UA, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
AU 9734063	A1	19980114	AU 1997-34063	19970620
AU 731925	B2	20010405		
EP 915876	A1	19990519	EP 1997-930167	19970620

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R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, SI, LT, LV, FI, RO

BR 9710087	A	19990810	BR 1997-10087		19970620
CN 1231666	A	19991013	CN 1997-197413		19970620
JP 2000510154	T2	20000808	JP 1998-503379		19970620
NZ 332605	A	20000929	NZ 1997-332605		19970620
KR 2000022297	A	20000425	KR 1998-710719		19981228
PRIORITY APPLN. INFO.:			US 1995-373132	A2	19950117
			US 1996-672150	A	19960627
			WO 1997-US10736	W	19970620

OTHER SOURCE(S): MARPAT 129:16148

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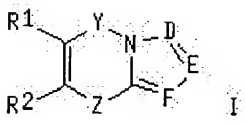

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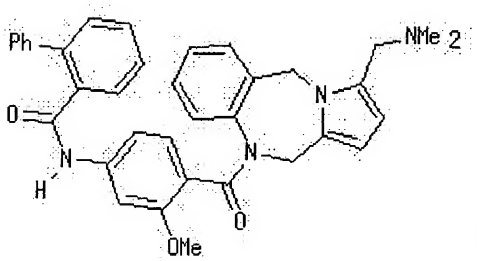

II

AB Title compds. [I; D,E,F = N or (un)substituted CH; R1R2 = atoms to complete an(un)substituted (hetero)arom. ring; Y = bond, CH2, CH2CH2, CO, alkylidene; Z = (CH2)mNR3 or NR3(CH2)m; R3 = CO2Z1R6; R6 = acylamino, etc.; Z1 = (un)substituted 1,4-phenylene or -3,6-pyridinediyl; m = 1 or 2] were prepd. Thus, 1-(2-nitrobenzyl)pyrrole-2-carboxaldehyde (prepn. given) was reductively cyclized and the product N-acylated by 2-PhC6H4CONHC6H4(OMe)(CO2H)-3,4 (prepn. given) to give, after condensation with HCHO/CH2(NMe2)2, title compd. II. Data for biol. activity of I were given.

IT **200878-81-5P**

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of tricyclic benzodiazepines as vasopressin antagonists)

RN 200878-81-5 HCAPLUS

CN Benzamide, N-[5-(5H-pyrrolo[2,1-c][1,4]benzodiazepin-10(11H)-ylcarbonyl)-2-pyridinyl]-2-(2-pyridinyl)- (9CI) (CA INDEX NAME)

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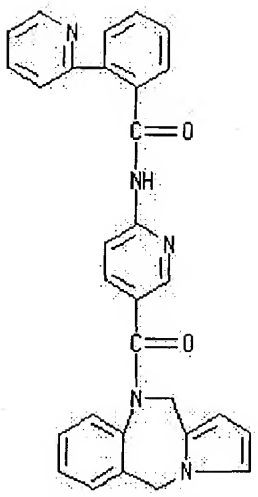

REFERENCE COUNT: 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 98 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 1998:8260 HCAPLUS
DOCUMENT NUMBER: 128:88934
TITLE: Preparation of tricyclic benzazepine vasopressin antagonists
INVENTOR(S): Albright, Jay Donald; Venkatesan, Aranapakam M.; Dusza, John P.; Sum, Fuk-wah
PATENT ASSIGNEE(S): American Cyanamid Co., USA
SOURCE: U.S., 64 pp., Cont.-in-part of U.S. 5,536,718. CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 4
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5700796	A	19971223	US 1996-671442	19960627
US 5536718	A	19960716	US 1995-373132	19950117
WO 9749708	A1	19971231	WO 1997-US10755	19970620
W: AL, AU, BA, BB, BG, BR, CA, CN, CU, CZ, EE, GE, GH, HU, IL, IS, JP, KP, KR, LC, LK, LR, LT, LV, MG, MK, MN, MX, NO, NZ, PL, RO, RU, SG, SI, SK, SL, TR, TT, UA, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
AU 9736414	A1	19980114	AU 1997-36414	19970620

PRIORITY APPLN. INFO.:

US 1995-373132	A2	19950117
US 1996-671442	A	19960627
WO 1997-US10755	W	19970620

OTHER SOURCE(S): MARPAT 128:88934
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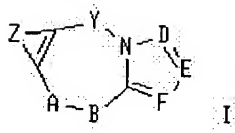

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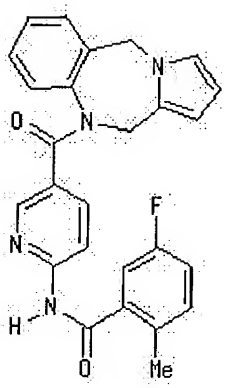


II

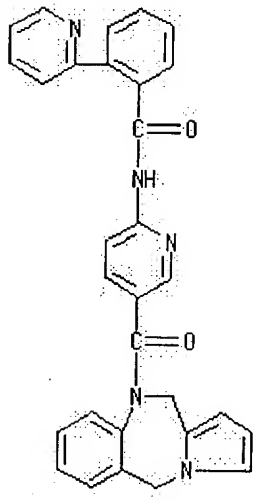
AB The title compds. [I; Y = (CH2)n (n = 0-2), CH(C1-3 alkyl), C(O); AB = (CH2)mNR3, NR3(CH2)m (m = 1-2; R3 = C(O)Ar; Ar = (un)substituted Ph, 3-pyridyl); Z with two carbon atoms attached = (un)substituted Ph, a 5-membered arom. heterocyclic ring having one heteroatom selected from O,N,S, a 6-membered arom. heterocyclic ring having one N atom, etc.; D, E, F = C, N], which exhibit antagonist activity at V1 and/or V2 receptors, in vivo vasopressin antagonist activity, and oxytocin antagonist activity, and are useful in treating diseases characterized by excess renal reabsorption of water, were prepd. Thus, treatment of 6-[(5-fluoro-2-methylbenzoyl)amino]pyridine-3-carboxylic acid with SOCl2 followed by reaction of the resulting acid chloride with 10,11-dihydro-5H-pyrrolo[2,1-c][1,4]benzodiazepine afforded the title compd. II which showed IC50 of 0.033 μM against rat hepatic V1 receptors binding and IC50 of 0.004 μM against rat kidney medullary V2 receptors binding.

IT **200878-81-5P**

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of tricyclic benzazepine vasopressin antagonists)

RN 200878-81-5 HCAPLUS

CN Benzamide, N-[5-(5H-pyrrolo[2,1-c][1,4]benzodiazepin-10(11H)-ylcarbonyl)-2-pyridinyl]-2-(2-pyridinyl)- (9CI) (CA INDEX NAME)



L12 ANSWER 99 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

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Full Text | Citing References

ACCESSION NUMBER: 1997:735797 HCAPLUS
DOCUMENT NUMBER: 128:22928
TITLE: Preparation of cyclic urea HIV protease inhibitors
INVENTOR(S): Jadhav, Prabhakar Kondaji; Ko, Soo Sung
PATENT ASSIGNEE(S): Dupont Merck Pharmaceutical Co., USA
SOURCE: U.S., 68 pp., Cont.-in-part of U.S. Ser. No. 406,240, abandoned.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5683999	A	19971104	US 1996-613554	19960311
CA 2215536	AA	19960926	CA 1996-2215536	19960313
WO 9629329	A1	19960926	WO 1996-US3426	19960313
W: AU, BR, CA, CN, CZ, EE, HU, JP, KR, LT, LV, MX, NO, NZ, PL, RO, SG, SI, SK, UA, VN, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
AU 9653100	A1	19961008	AU 1996-53100	19960313
EP 815108	A1	19980107	EP 1996-909680	19960313
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE				
ZA 9602133	A	19970915	ZA 1996-2133	19960315
PRIORITY APPLN. INFO.:			US 1995-406240	B2 19950317
			US 1996-613554	A 19960311
			WO 1996-US3426	W 19960313

OTHER SOURCE(S): MARPAT 128:22928
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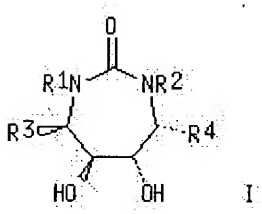


I

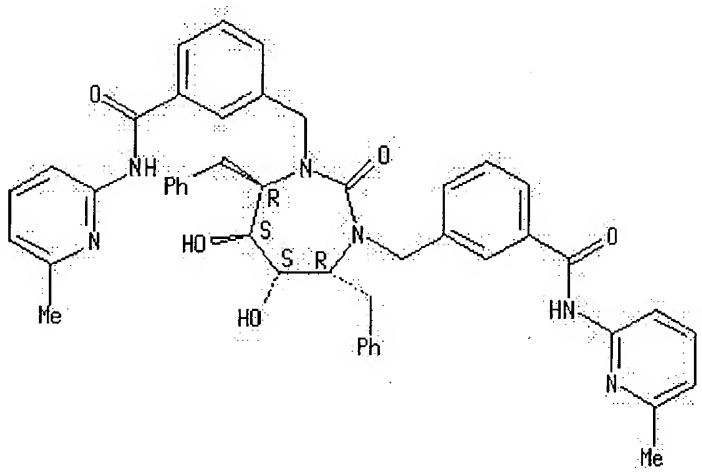
AB Cyclic ureas I [R1 = CH2XYZ; X = alkyl, aryl, cycloalkyl, etc.; Y = (CH2)nO, (CH2)nS, (CH2)nC(:NH)NH, etc.; n = 0-2; Z = 2-, 3-, or 4-pyridyl, 2-pyrazinyl, etc.; R2 = R1, CH2XY1Z1, H, etc. Y1 = (CH2)nO(CH2)m, (CH2)nS(CH2)m, etc.; Z1 = H, alkyl, alkenyl, aryl, etc.; R3, R4 = benzyl, 2-pyrrolylmethyl, Et, iso-Bu, hexyl, etc.] useful as inhibitors of HIV protease (no data), were prepd. The present invention also relates to pharmaceutical compns. comprising such compds. and to method of using these compds. for the treatment HIV infection. The present invention also relates to the use of such compds. in processes for the identification of HIV protease inhibitors and for the inhibition or detection of HIV in a bodily fluid sample (no data).

IT **183854-97-9P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of cyclic urea HIV protease inhibitors)

h eb c g cg b cg eb

RN 183854-97-9 HCAPLUS
CN Benzamide, 3,3'-[[(4R,5S,6S,7R)-tetrahydro-5,6-dihydroxy-2-oxo-4,7-bis(phenylmethyl)-1H-1,3-diazepine-1,3(2H)-diyl]bis(methylene)]bis[N-(6-methyl-2-pyridinyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L12 ANSWER 100 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 1997:727376 HCAPLUS
DOCUMENT NUMBER: 128:30079
TITLE: Nonsymmetrically Substituted Cyclic Urea HIV Protease Inhibitors
AUTHOR(S): Wilkerson, Wendell W.; Dax, Scott; Cheatham, Walter W.
CORPORATE SOURCE: DuPont Merck Pharmaceutical Company, Wilmington, DE, 19880-0500, USA
SOURCE: Journal of Medicinal Chemistry (1997), 40(25), 4079-4088
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

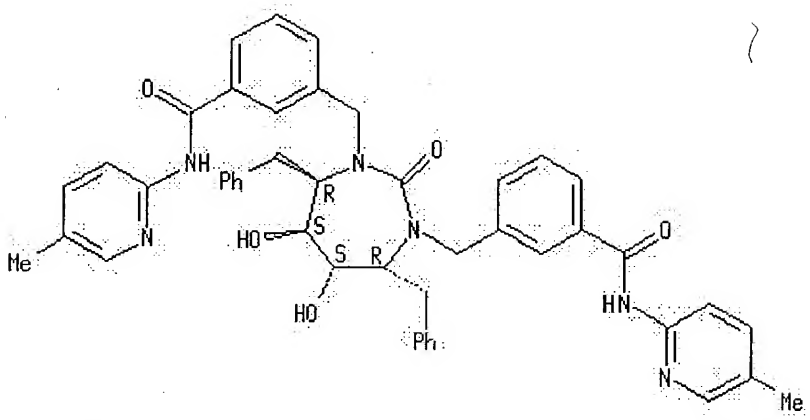
AB A series of nonsym. substituted cyclic urea carboxamides was synthesized and evaluated for antiviral activity as a function of the inhibition of HIV-protease. Selected protease inhibitors were also evaluated for oral bioavailability. The synthesis, pharmacol., quant. structure-activity relationship (QSAR), and pharmacokinetics for the series will be discussed.

IT **199738-20-0P**
RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); PROC (Process)
(prepn. of substituted cyclic ureas as HIV protease inhibitors)

RN 199738-20-0 HCAPLUS
CN Benzamide, 3,3'-[[tetrahydro-5,6-dihydroxy-2-oxo-4,7-bis(phenylmethyl)-1H-1,3-diazepine-1,3(2H)-diyl]bis(methylene)]bis[N-(5-methyl-2-pyridinyl)-, (4α,5α,6β,7β)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

h eb c g cg b cg eb



REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 101 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 1997:499168 HCAPLUS
DOCUMENT NUMBER: 127:190649
TITLE: Preparation of 9-aralkyl-9-fluorenecarboxamides and analogs as microsomal triglyceride transfer protein inhibitors
INVENTOR(S): Biller, Scott A.; Dickson, John K.; Lawrence, R. Michael; Magnin, David R.; Poss, Michael A.; Robl, Jeffrey A.; Slusarchyk, William A.; Sulsky, Richard B.; Tino, Joseph A.
PATENT ASSIGNEE(S): Bristol-Myers Squibb Co., USA
SOURCE: PCT Int. Appl., 615 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9726240	A1	19970724	WO 1997-US587	19970113
W: AL, AM, AT, AU, AZ, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TR, TT, UA, UG, UZ, VN, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
CA 2236684	AA	19970724	CA 1997-2236684	19970113
AU 9718285	A1	19970811	AU 1997-18285	19970113
AU 716729	B2	20000302		
CN 1209803	A	19990303	CN 1997-191713	19970113
EP 904262	A1	19990331	EP 1997-903805	19970113
EP 904262	B1	20040421		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
BR 9707607	A	19990727	BR 1997-7607	19970113
JP 2000502355	T2	20000229	JP 1997-526127	19970113
NZ 330216	A	20000929	NZ 1997-330216	19970113
AT 264833	E	20040515	AT 1997-903805	19970113

h eb c g cg b cg eb

ZA 9700328	A	19970715	ZA 1997-328		19970115
NO 9803268	A	19980715	NO 1998-3268		19980715
PRIORITY APPLN. INFO.:			US 1996-10346P	P	19960116
			US 1996-17224P	P	19960509
			US 1996-30370P	P	19961105
			WO 1997-US587	W	19970113

OTHER SOURCE(S): MARPAT 127:190649

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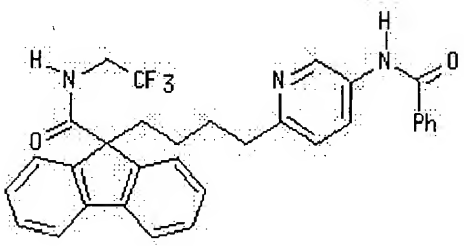


I

AB R2Z4Z3ZZ2Z1R1 [R1 = H, (cyclo)alk(en)yl, alkoxy, (hetero)aryl(oxy), etc.; R2 = groups cited for R1, haloalkyl, etc.; Z = CO, SO0-2, CR(OH); R = H, alkyl, aryl; Z1 = (O- or NH-interrupted)(oxo)alk(en)ylene, etc.; Z2 = (un)substituted 9H-fluoren-9-ylidene, 9H-xanthen-9-ylidene, etc.; Z3 = bond, O, NR5; R5 = H or alkyl; R2R5 = atoms to form a ring; Z4 = bond, groups cited for Z1] were prepd as microsomal triglyceride transfer protein inhibitors (no data). Thus, 9H-fluorene-9-carboxylic acid was alkylated by TsOCH2CH2C≡CH and the product amidated by H2NCH2CF3 9-(3-butynyl)-N-(2,2,2-trifluoroethyl)fluorene-9-carboxamide which was arylated by 2-bromo-5-nitropyridine to give, after redn. and BzCl amidation, title compd. I.

IT **194214-02-3P**

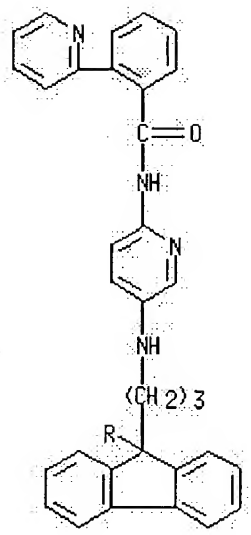
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of 9-aralkyl-9-fluorenecarboxamides and analogs as microsomal triglyceride transfer protein inhibitors)

RN 194214-02-3 HCAPLUS

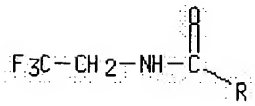
CN 9H-Fluorene-9-carboxamide, 9-[3-[[6-[[2-(2-pyridinyl)benzoyl]amino]-3-pyridinyl]amino]propyl]-N-(2,2,2-trifluoroethyl)-, dihydrochloride (9CI) (CA INDEX NAME)

h eb c g cg b cg eb

PAGE 1-A



PAGE 2-A



2 HCl

L12 ANSWER 102 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 1997:261509 HCAPLUS
DOCUMENT NUMBER: 127:28386
TITLE: Selective membrane transport of dicarboxylic acids in their neutral form by a synthetic receptor containing amidopyridine groups
AUTHOR(S): Palet, Cristina; Munoz, Maria; Valiente, Manuel; Cynkowski, Tadeusz; Daunert, Sylvia; Bachas, Leonidas G.
CORPORATE SOURCE: Quimica Analitica, Universitat Autonoma de Barcelona, 08193 Bellaterra, Barcelona, Spain
SOURCE: Analytica Chimica Acta (1997), 343(3), 287-294
CODEN: ACACAM; ISSN: 0003-2670
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A synthetic receptor that can discriminate dicarboxylic acids based on host-guest principles was prepd. This compd. incorporates two amidopyridine units as hydrogen-bonding centers that are capable of binding the carboxylic acid functional group. The receptor was dissolved in a kerosine/dodecanol mixt. and used as a carrier in supported liq. membranes. Facilitated transport based on the liq.-liq. distribution of dicarboxylic acids between aq. feed and stripping solns. and an org. phase contg. the carrier was accomplished. This transport was driven by a pH gradient that assures the predominance of the protonated neutral form of the carboxylic acids in the feed soln. and the corresponding deprotonated

h eb c g cg b cg eb

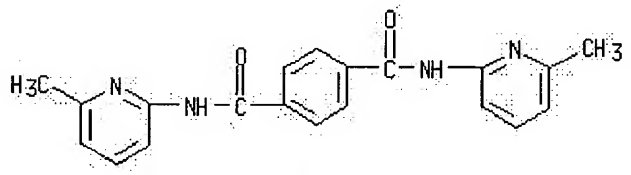
form in the stripping soln. Selective transport of dicarboxylic acids was obsd. allowing for an efficient sepn. of different carboxylic acids.

IT **129708-38-9P**

RL: PEP (Physical, engineering or chemical process); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)
(selective membrane transport of dicarboxylic acids in their neutral form by using synthetic receptor contg. amidopyridine groups)

RN 129708-38-9 HCAPLUS

CN 1,4-Benzenedicarboxamide, N,N'-bis(6-methyl-2-pyridinyl)- (9CI) (CA INDEX NAME)



L12 ANSWER 103 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 1997:256031 HCAPLUS
DOCUMENT NUMBER: 126:343288
TITLE: Molecular recognition: a simple dinaphthyridine receptor for urea. [Erratum to document cited in CA126:277143]
AUTHOR(S): Goswami, S.; Mukherjee, R.
CORPORATE SOURCE: Dep. Chem., Indian Inst. Technol., Kharagpur, 721302, India
SOURCE: Tetrahedron Letters (1997), 38(14), 2391
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English

AB On page 1621, in the eleventh line, 2-Oxobutyryldehyde should read 3-Oxobutyryldehyde. On page 1622, in ref. 14, the year should be 1965, not 1995.

IT **188916-88-3**

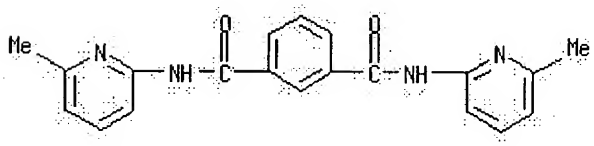
RL: FMU (Formation, unclassified); PRP (Properties); FORM (Formation, nonpreparative)
(NMR of truncated bipyridyl receptor complex with urea and imidazolidinone (Erratum))

RN 188916-88-3 HCAPLUS

CN 1,3-Benzenedicarboxamide, N,N'-bis(6-methyl-2-pyridinyl)-, compd. with 2-imidazolidinone (1:1) (9CI) (CA INDEX NAME)

CM 1

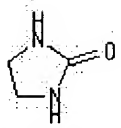
CRN 130760-57-5
CMF C20 H18 N4 O2



CM 2

h eb c g cg b cg eb

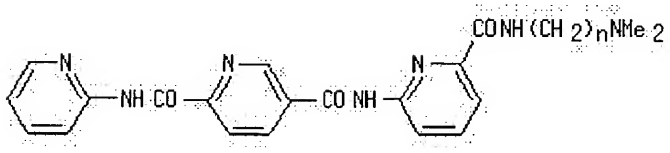
CRN 120-93-4
CMF C3 H6 N2 O



L12 ANSWER 104 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 1997:232915 HCAPLUS
DOCUMENT NUMBER: 126:293206
TITLE: Synthetic analogs of netropsin and distamycin. I. Pyridine-containing analogs of distamycin - a molecular modeling study
AUTHOR(S): Bielawski, Krzysztof; Bartulewicz, Danuta; Rozanski, Andrzej
CORPORATE SOURCE: Department of Organic Chemistry, Institute of Chemistry, Medical Academy of Bialystok, Pol.
SOURCE: Roczniki Akademii Medycznej w Bialymstoku (1995), 40(2), 352-363
CODEN: RAMBFJ
PUBLISHER: Akademia Medyczna w Bialymstoku
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

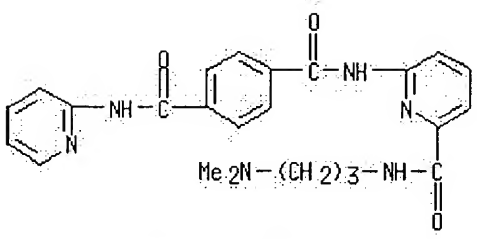


I

AB A new series of pyridine-contg. analogs of distamycin A were investigated by mil. modeling. Mol. mechanics techniques revealed evident structural similarities between analogs I [X = N, CH; n = 2, 3] and pyridine-2-carboxamide-netropsin, suggesting possible interactions of these compds. with DNA. Mol. modeling to the B-DNA d(CGCAGCTTTGCG) duplex shows that I [X = N, n = 3, II] fits tightly into the minor groove. The pattern of hydrogen bonds in the computed complex covers C6·G19, T7·A18, T8·A17, and T9·A16. The most striking feature of the II·DNA (1:1) complex is the recognition of the guanine amino group (G19) by the pyridine nitrogen of II.

IT **189000-55-3**
RL: PRP (Properties)
(mol. modeling study of pyridine-contg. analogs of distamycin)
RN 189000-55-3 HCAPLUS
CN 1,4-Benzenedicarboxamide, N-[6-[[[3-(dimethylamino)propyl]amino]carbonyl]-2-pyridinyl]-N'-2-pyridinyl- (9CI) (CA INDEX NAME)

h eb c g cg b cg eb



L12 ANSWER 105 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 1997:231030 HCAPLUS
DOCUMENT NUMBER: 126:271318
TITLE: Assembling Organic Receptors around Transition Metal Templates: Functionalized Catechols and Dioxomolybdenum(VI) for the Recognition of Dicarboxylic Acids
AUTHOR(S): Prevot-Halter, Isabelle; Smith, Thomas J.; Weiss, Jean
CORPORATE SOURCE: Laboratoire d'Electrochimie Faculte de Chimie, URA no. 405 au CNRS Universite Louis Pasteur, Strasbourg, F-67000, Fr.
SOURCE: Journal of Organic Chemistry (1997), 62(7), 2186-2192
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The synthesis of two receptors for dicarboxylic acids MoO2(1)2 [12]2- and MoO2(2)2 [13]2-, based on the self arrangement of two functionalized catechols (OH)2C6H3(p- or m-)C6H4CONH(C5H3N)Me 1 or 2 around a cis-[MoO2]2- core, is described. Among the three pairs of enantiomers which may be produced during the complexation of two unsym. catecholates around one Mo(IV) ion, only one is obsd. for each catechol deriv. 1 or 2. Depending on the base used during the complexation of catechols to the Mo atom, the dianionic receptors obtained display different soly. properties. These Mo-based receptors are chromogenic and, in CH2Cl2, the affinities of the assembled receptors for dicarboxylic acids ranging from C4 to C8 were assessed by UV-visible titrns. after detg. the stoichiometry of the complex formation using Job's method. While receptor [12]2- displays selectivity for C4 and C5 acids, the more flexible receptor [13]2- exhibits selectivity for C7 and C8. The binding mode of the diacids to the Mo receptor was detd. based on 1H NMR titrn. Due to the intrinsic chirality of the receptors, their binding properties vs. chiral dicarboxylic acid were examd. The enantioselective binding of N-Cbz protected L and D-glutamic acid due to addnl. π-π interactions of the protecting group with the receptor's framework is reported for [12]2- in CH2Cl2. For comparison, the assocn. consts. of receptor [12]2- with a Boc protected L-glutamic acid and the racemic mixt. of N-carbobenzyloxy protected glutamic acid were detd.

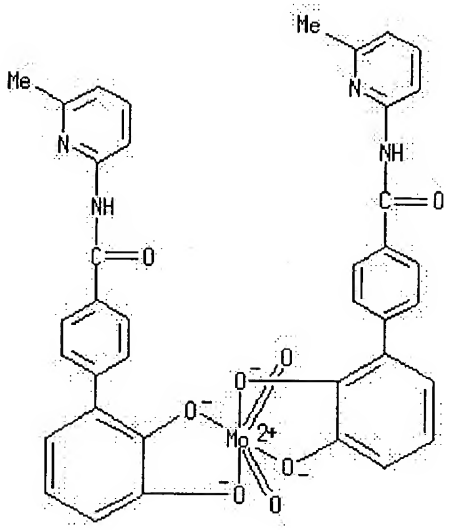
IT **174878-42-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(mol. recognition of dicarboxylic acids by dioxomolybdenum complexes of functionalized catechols)

RN 174878-42-3 HCAPLUS
CN 1-Butanaminium, N,N,N-tributyl-, (OC-6-33)-bis[2',3'-di(hydroxy-κO)-N-(6-methyl-2-pyridinyl)[1,1'-biphenyl]-4-carboxamidato(2-)]dioxomolybdate(2-) (2:1) (9CI) (CA INDEX NAME)

CM 1

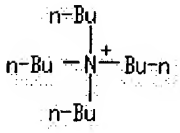
h eb c g cg b cg eb

CRN 174878-41-2
CMF C38 H28 Mo N4 O8
CCI CCS



CM 2

CRN 10549-76-5
CMF C16 H36 N



L12 ANSWER 106 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER:	1997:169822 HCAPLUS
DOCUMENT NUMBER:	126:277143
TITLE:	Molecular recognition: a simple dinaphthyridine receptor for urea
AUTHOR(S):	Goswami, Shyamprosad; Mukherjee, Rakhi
CORPORATE SOURCE:	Dep. Chem., Indian Inst. Technol., Kharagpur, 721302, India
SOURCE:	Tetrahedron Letters (1997), 38(9), 1619-1622 CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER:	Elsevier
DOCUMENT TYPE:	Journal
LANGUAGE:	English
GI	

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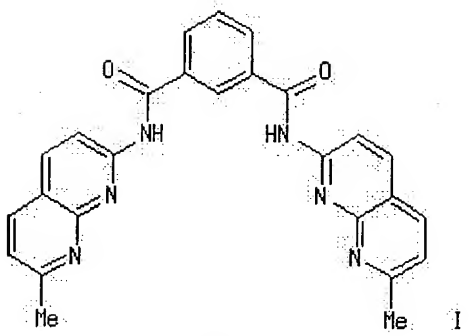
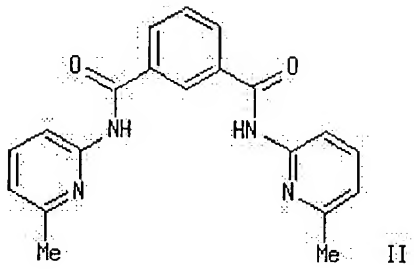


I



II

AB A new dinaphthyridine receptor I is designed that efficiently binds to urea probably by six hydrogen bonds forming a chloroform sol. 1:1 complex and selectively exts. urea into chloroform from its mixt. with thiourea. The receptor I has fifteen fold higher binding const. for urea than the truncated receptor II possibly due to formation of greater no. of hydrogen bonds in complexation.

IT **188916-88-3**

RL: FMU (Formation, unclassified); PRP (Properties); FORM (Formation, nonpreparative)

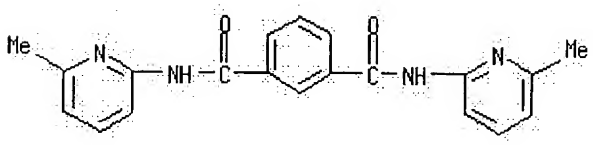
(NMR of truncated bipyridyl receptor complex with urea and imidazolidinone)

RN 188916-88-3 HCAPLUS

CN 1,3-Benzenedicarboxamide, N,N'-bis(6-methyl-2-pyridinyl)-, compd. with 2-imidazolidinone (1:1) (9CI) (CA INDEX NAME)

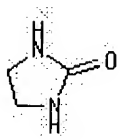
CM 1

CRN 130760-57-5
CMF C20 H18 N4 O2



CM 2

CRN 120-93-4
CMF C3 H6 N2 O



h eb c g cg b cg eb

REFERENCE COUNT: 42 THERE ARE 42 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 107 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 1997:168937 HCAPLUS
DOCUMENT NUMBER: 126:231713
TITLE: X-ray structure of the 1:1 complex of a tripodal receptor and cis-cyclohexane-1,3,5-tricarboxylic acid
AUTHOR(S): Ballester, Pablo; Costa, Antoni; Deya, Pere M.; Deslongchamps, Ghislain; Mink, Daniel; Decken, Andreas; Prohens, Rafael; Tomas, Salvador; Vega, Manuel
CORPORATE SOURCE: Dep. Quim., Univ. de les Illes Balears, Palma de Mallorca, 07071, Spain
SOURCE: Chemical Communications (Cambridge) (1997), (4), 357-358
CODEN: CHCOFS; ISSN: 1359-7345
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The x-ray crystal structure of 1:1 complex of a tripodal abiotic receptor and cis-cyclohexane-1,3,5-tricarboxylic acid is reported; the 1:1 complex is devoid of C3-symmetry and packs into a multi-columnar self-assembly. Crystallog. data are given.

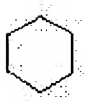
IT **188303-33-5**
RL: PRP (Properties)
(crystal structure of)

RN 188303-33-5 HCAPLUS

CN 1,3,5-Cyclohexanetricarboxylic acid, (1α,3α,5α)-, compd. with cyclohexane and 4,4''-dihydroxy-5'-[4-hydroxy-3-[[(6-methyl-2-pyridinyl)amino]carbonyl]-5-propylphenyl]-N,N'-bis(6-methyl-2-pyridinyl)-5,5''-dipropyl[1,1':3',1''-terphenyl]-3,3''-dicarboxamide (2:1:2) (9CI) (CA INDEX NAME)

CM 1

CRN 110-82-7
CMF C6 H12

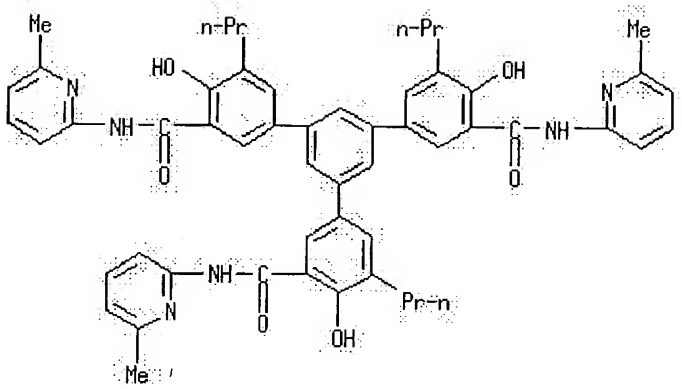


CM 2

CRN 157460-61-2
CMF C54 H54 N6 O6 . C9 H12 O6

CM 3

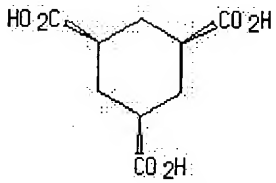
CRN 157460-60-1
CMF C54 H54 N6 O6



CM 4

CRN 16526-68-4
CMF C9 H12 O6

Relative stereochemistry.



REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 108 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | CAS Ring References

ACCESSION NUMBER: 1996:751515 HCAPLUS
DOCUMENT NUMBER: 126:18896
TITLE: preparation of cyclic urea derivatives as HIV protease inhibitors
INVENTOR(S): Jadhav, Prabhakar Kondaji
PATENT ASSIGNEE(S): E. I. Du Pont de Nemours & Co., USA
SOURCE: PCT Int. Appl., 195 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

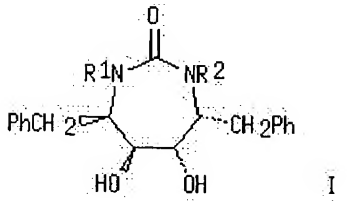
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9629329	A1	19960926	WO 1996-US3426	19960313
W: AU, BR, CA, CN, CZ, EE, HU, JP, KR, LT, LV, MX, NO, NZ, PL, RO, SG, SI, SK, UA, VN, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
US 5683999	A	19971104	US 1996-613554	19960311
AU 9653100	A1	19961008	AU 1996-53100	19960313
EP 815108	A1	19980107	EP 1996-909680	19960313
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE				

PRIORITY APPLN. INFO.:

US 1995-406240	A	19950317
US 1996-613554	A	19960311
WO 1996-US3426	W	19960313

h eb c g cg b cg eb

OTHER SOURCE(S): MARPAT 126:18896
GI



I

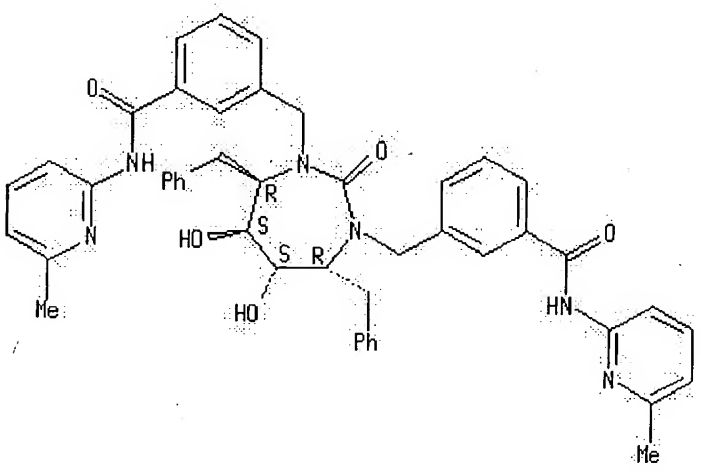
AB The title compds. [I; R1 = heterocyclylmethyl; R2 = H, R1], useful as HIV protease inhibitors and thus effective in treating HIV infections, are prepd. and formulated. I are effective at 1.0-20 mg/kg-day p.o. Capsule, injectable, etc. formulations were given.

IT **183854-97-9P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of cyclic urea derivs. as HIV protease inhibitors)

RN 183854-97-9 HCAPLUS

CN Benzamide, 3,3'-[[(4R,5S,6S,7R)-tetrahydro-5,6-dihydroxy-2-oxo-4,7-bis(phenylmethyl)-1H-1,3-diazepine-1,3(2H)-diyl]bis(methylene)]bis[N-(6-methyl-2-pyridinyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L12 ANSWER 109 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 1996:618915- HCAPLUS
DOCUMENT NUMBER: 126:8087
TITLE: HIV Protease Inhibitory Bis-benzamide Cyclic Ureas: A Quantitative Structure-Activity Relationship Analysis
AUTHOR(S): Wilkerson, Wendell W.; Akamike, Emeka; Cheatham, Walter W.; Hollis, Andrea Y.; Collins, R. Dale; DeLucca, Indawati; Lam, Patrick Y. S.; Ru, Yu
CORPORATE SOURCE: Chemical and Physical Sciences, DuPont Merck Pharmaceutical Company, Wilmington, DE, 19880-0500, USA
SOURCE: Journal of Medicinal Chemistry (1996), 39(21), 4299-4312

h eb c g cg b cg eb

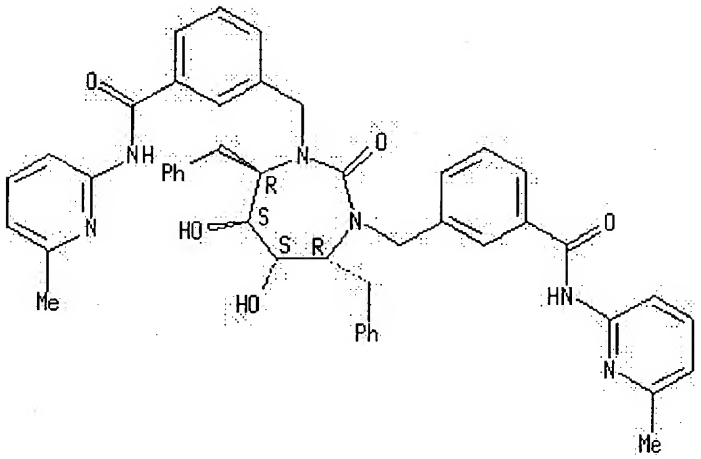
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A series of N,N'-disubstituted cyclic urea 3-benzamides has been synthesized and evaluated for HIV protease inhibition and antiviral activity. Some of these benzamides have been shown to be potent inhibitors of HIV protease with Ki < 0.050 nM and IC90 < 20 nM for viral replication and, as such, may be useful in the treatment of AIDS. The synthesis and quant. structure-activity relationship for this benzamide series will be discussed.

IT **183854-97-9P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(prepn. and QSAR of HIV protease inhibitory bis-benzamide cyclic ureas)

RN 183854-97-9 HCAPLUS
CN Benzamide, 3,3'-[[(4R,5S,6S,7R)-tetrahydro-5,6-dihydroxy-2-oxo-4,7-bis(phenylmethyl)-1H-1,3-diazepine-1,3(2H)-diyl]bis(methylene)]bis[N-(6-methyl-2-pyridinyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L12 ANSWER 110 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 1996:373467 HCAPLUS
DOCUMENT NUMBER: 125:56131
TITLE: Seleno-organic compounds as immunostimulants: An approach to the structure-activity relationship
AUTHOR(S): Inglot, Anna D.; Mlochowski, Jacek; Zielinska-Jenczylik, Janina; Piasecki, Egbert; Ledwon, Tomasz K.; Kloc, Krystian
CORPORATE SOURCE: Institute Immunology and Experimental Therapy, Polish Academy Sciences, Wroclaw, 53-114, Pol.
SOURCE: Archivum Immunologiae et Therapiae Experimentalis (1996), 44(1), 67-75
CODEN: AITEAT; ISSN: 0004-069X
PUBLISHER: Zaklad Narodowy imienia Ossolinskich
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Our studies on the seleno-org. compds. were focused at their activities as modest cytokine inducers in human peripheral blood leukocyte cultures.

h eb c g cg b cg eb

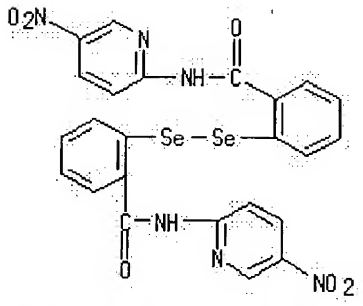
Our bioassays used in the screening methods were based on the quant. detns. of mainly two types of cytokines: interferons (IFNs) and tumor necrosis factors (TNFs). More recently we have found that several of the compds. have direct immunotropic actions in vitro and in vivo, in mice and in chickens. The paper summarizes the data related to the cytokine-inducing activity of 65 seleno-org. compds. divided into 4 groups according to their chem. structures. The ref. compd. was ebselen, the well known exptl. drug with various biol. activities. Approx. 50% of the compds. were found to be active in our bioassays. The selected compds. induced also IL-6 and GM-CSF. Their activities were clearly correlated with defined chem. structures as well as with the presence of selenium. We suggest that some of the compds., other than ebselen, are interesting as immunostimulants and potential antiviral agents and cytokine inducers active in humans.

IT **175612-99-4**

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(antiviral, cytokine-inducing, and tumor cytotoxic activities of seleno-org. compds.)

RN 175612-99-4 HCAPLUS

CN Benzamide, 2,2'-diselenobis[N-(5-nitro-2-pyridinyl)- (9CI) (CA INDEX NAME)



L12 ANSWER 111 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Ref References

ACCESSION NUMBER:	1996:166637 HCAPLUS
DOCUMENT NUMBER:	124:278400
TITLE:	Immunotropic activities of benzisoselenazolones and organic diselenides in mice
AUTHOR(S):	Blaszczyk, Barbara; Inglot, Anna D.; Kowalczyk-Bronisz, Stefania H.; Szymaniec, Stanislaw; Mlochowski, Jacek
CORPORATE SOURCE:	Institute Immunology and Experimental Therapy, Polish Academy Sciences, Wroclaw, 53-114, Pol.
SOURCE:	Archivum Immunologiae et Therapiae Experimentalis (1995), 43(5-6), 305-11 CODEN: AITEAT; ISSN: 0004-069X
PUBLISHER:	Zaklad Narodowy imienia Ossolinskich
DOCUMENT TYPE:	Journal
LANGUAGE:	English

AB We have investigated the immunotropic effects of 23 seleno-org. compds. (8 benzisoselenazolones, 3 benzisoselenazolone oxides and 12 org. diselenides). All of the compds. increased the rosette formation of sheep red blood cells (SRBC) with spleen cells obtained from thymectomized C53BL/6 mice and incubated in vitro in the presence of imuran. Furthermore, 16 of the compds. were also assayed in vitro in the hydrocortisone test performed with C57BL/6 mouse thymocytes. It was found

h eb c g cg b cg eb

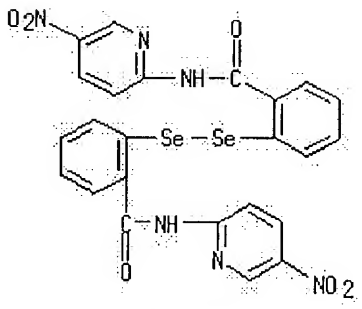
that all of them significantly protected the cells against hydrocortisone-induced cytotoxicity. Also in the Jerne's assay, performed in 129Ao/Boy mice pretreated in vivo with 3 selected compds. 5 days before immunization with SRBC, the stimulation of plaque forming cells (PFC) was obsd. Only one compd. (AE22, an analog of piroxicam) was found to be inhibitory in this assay. In contrast, in the graft vs. host (GvH) assay performed in hybrid mice the donor lymphoid cells obtained from C57BL/6 mice pretreated with 9 selected seleno-org. compds., suppressed the GvH reaction in the recipient hybrid mice. Thus, in all of the immunotropic assays except the GvH reaction in adult mice, the seleno-org. compds. were found to have immunostimulating activities.

IT **175612-99-4**

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(seleno-org. compds. immunostimulant activity)

RN 175612-99-4 HCAPLUS

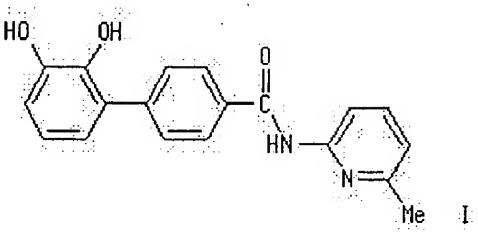
CN Benzamide, 2,2'-diselenobis[N-(5-nitro-2-pyridinyl)- (9CI) (CA INDEX NAME)



L12 ANSWER 112 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 1996:132012 HCAPLUS
DOCUMENT NUMBER: 124:248771
TITLE: Synthesis of a dicarboxylic acid receptor organized around a dioxomolybdenum core
AUTHOR(S): Prevot-Halter, Isabelle; Smith, Thomas J.; Weiss, Jean
CORPORATE SOURCE: Faculte Chimie, Univ. Louis Pasteur, Strasbourg, 67000, Fr.
SOURCE: Tetrahedron Letters (1996), 37(8), 1201-4
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



AB Reaction of bis(acetylacetonato)dioxomolybdenum with 2 equiv 4-(2,3-dihydroxyphenyl)benzoyl 6-methyl-2-pyridylamide (I, H2L, prepn.

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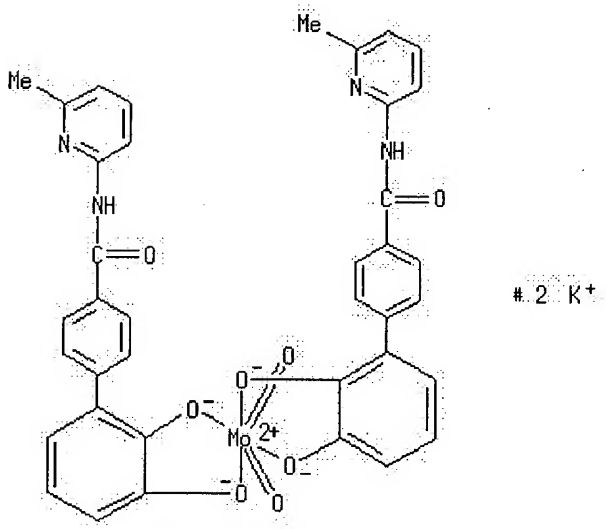
given) in EtOH in the presence of base afforded catecholate complexes K2[MoO2L2] or (Bu4N)2[MoO2L2]. Only one pair of enantiomers of [MoO2L2]2- out of three possible was obtained. The receptor characteristics of catecholate complexes K2[MoO2L2] and (Bu4N)2[MoO2L2] for dicarboxylic acids were studied; binding consts. were detd. from UV-visible titrn. curves, and the 1:1 stoichiometry of the complex formation was confirmed by Job's method. Despite the relative rigidity of the [MoO2L2]2- framework, only a slight preference for HO2C(CH2)nCO2H (n = 2, 3) was noticeable. This work expands the concept of assembling receptors around metal templates to metal binding groups other than polyimine ligands.

IT **174878-40-1P**

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(prepn. as receptor for dicarboxylic acids)

RN 174878-40-1 HCAPLUS

CN Molybdate(2-), bis[2',3'-dihydroxy-N-(6-methyl-2-pyridinyl)[1,1'-biphenyl]-4-carboxamidato(2-)-O2',O3']dioxo-, dipotassium, (OC-6-33)- (9CI) (CA INDEX NAME)



L12 ANSWER 113 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Cited References

ACCESSION NUMBER:	1995:834662 HCAPLUS
DOCUMENT NUMBER:	124:56600
TITLE:	Chiral 1,1'-binaphthyl molecular clefts for the complexation of excitatory amino-acid derivatives
AUTHOR(S):	Martinborough, Esther; Denti, Tiziana Modasini; Castro, Peter P.; Wyman, Tara B.; Knobler, Carolyn B.; Diederich, Francois
CORPORATE SOURCE:	Lab. Org. Chem., Eidgenoessichen Tech. Hocheschule, Zurich, CH08092, Switz.
SOURCE:	Helvetica Chimica Acta (1995), 78(5), 1037-66 CODEN: HCACAV; ISSN: 0018-019X
PUBLISHER:	Verlag Helvetica Chimica Acta
DOCUMENT TYPE:	Journal
LANGUAGE:	English
OTHER SOURCE(S):	CASREACT 124:56600
GI	

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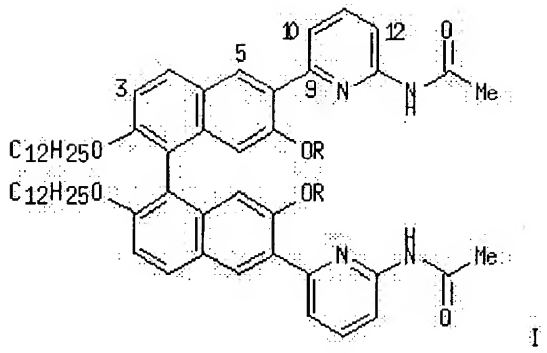

I

AB The complexation of N-Cbz derivs. of Asp, Glu, and L-kainic acid was studied in CDCl3 with various chiral receptors consisting of a 1,1'-binaphthyl spacer with (carboxamido)pyridine functionality at the 6,6'-positions in the major groove. Receptors of type A possess 2 N-(pyridin-2-yl)carboxamide H-bonding sites, whereas type B-receptors have 2 N-(pyridine-2,6-diyl)acetamide residues attached. Complexes of excitatory amino-acid derivs. and other, achiral α,ω-dicarboxylic acids with these receptors are primarily stabilized by 2 sets of C:O···H-N and O-H···N H-bonds. Optically active type-A receptors showed a preference for the large Glu deriv., whereas type-B receptors formed more stable complexes with the smaller Cbz-Asp. To improve the poor enantioselectivity addnl. functionality was introduced at the 7,7'-positions of the 1,1'-binaphthyl spacer, and the nature of the H-bonding sites in the 6,6'-positions was varied. (±)-I [R = CH2Ph, Me] formed the most stable complexes with dicarboxylic acids, and these receptors were synthesized in enantiomerically pure form. By 1H NMR binding titrns., the complexation of (R)- and (S)-I with the excitatory amino-acid derivs. was studied in CDCl3, and assocn. consts. of Ka = 103 - 2 105 ı L·mmol-1 were measured for the 1:1 host-guest complexes. Enantioselective binding was limited to I [R = CH2Ph], with the (R)-enantiomer complexing Cbz-Asp by 0.7 kcal·mol-1 more tightly than the (S)-enantiomer. An unusual variety of interesting arom. interactions and secondary electrostatic interactions are responsible for the high binding affinity and the enantioselection obsd. with (R)- and (S)-I [R = CH2Ph]. To enhance the enantioselectivity by reducing the conformational flexibility of the 1,1'-binaphthyl spacer, an addnl. crown-ether binding site was attached to the 2,2'-positions in the minor groove of type-B receptors. The binding affinity and the enantioselectivity were not altered upon complexation of Hg(CN)2 at the crown-ether binding site, demonstrating lack of cooperativity between the minor- and major-groove recognition sites.

IT **147650-11-1P**

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (assocn. consts. and prepn. of chiral 1,1'-binaphthyl mol. clefts with α,ω-dicarboxylic acid recognition sites)

RN 147650-11-1 HCAPLUS

CN Butanedioic acid, 2,2-diphenyl-, compd. with N,N'-bis(6-methyl-2-pyridinyl)-2,2'-bis(phenylmethoxy)[1,1'-binaphthalene]-6,6'-dicarboxamide (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 147650-10-0
CMF C48 H38 N4 O4

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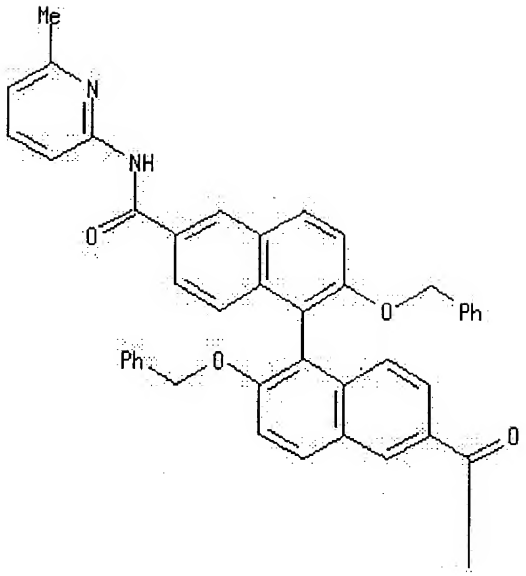
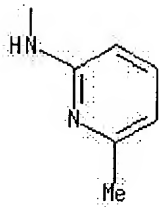
PAGE 1-A

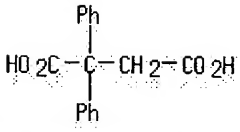


PAGE 2-A



CM 2

CRN 10186-26-2
CMF C16 H14 O4



L12 ANSWER 114 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 1995:714291 HCAPLUS
DOCUMENT NUMBER: 123:186781
TITLE: Self-Assembling, Chromogenic Receptors for the Recognition of Dicarboxylic Acids
AUTHOR(S): Goodman, M. Scott; Hamilton, Andrew D.; Weiss, Jean
CORPORATE SOURCE: Department of Chemistry, University of Pittsburgh, Pittsburgh, PA, 15260, USA
SOURCE: Journal of the American Chemical Society (1995), 117(32), 8447-55
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal

h eb c g cg b cg eb

LANGUAGE: English

AB The synthesis of 2 ligands (2,9-disubstituted phenanthrolines) bearing one or two acylaminopyridine binding sites (1 and 2, resp.) is described. Each ligand can assemble on a Cu(I) template, forming two different receptors for dicarboxylic acids, Cu(1)2+BF4- and Cu(2)2+BF4-. These orange Cu(I) complexes bind (Ka > 104 M-1) to a variety of dicarboxylic acids in CHCl3, with a slight preference for the C5-dicarboxylic acids, glutaric and N-CBz-glutamic acids, over shorter and longer substrates. Complexation is analyzed both by NMR chem. shift changes and UV-visible absorption changes. The data indicate formation of 1:1 complexes for Cu(1)2+BF4- and 2:1 complexes for Cu(2)2+BF4-, with the dicarboxylic acid substrate H bonding simultaneously to an acylaminopyridine binding site on each ligand. For Cu(2)2+BF4-, the complexation event results in large shifts in the visible absorption bands and a color change from orange to red. The change in the visible absorbance, and therefore the chromogenicity, is substrate dependent. The chromogenic effect is explained as being the result of a conformational change in the receptors resulting from H bond formation with the substrate.

IT **160473-37-0P**

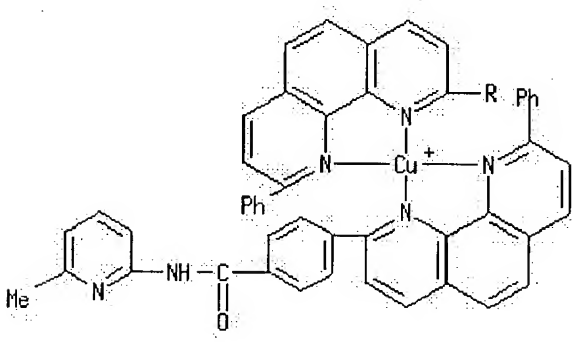
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and chromogenic reaction with dicarboxylic acids)

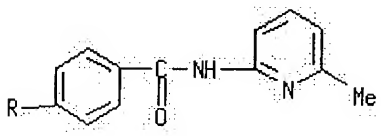
RN 160473-37-0 HCAPLUS

CN Copper(1+), bis[N-(6-methyl-2-pyridinyl)-4-(9-phenyl-1,10-phenanthrolin-2-yl)benzamide-N4,N4']-, (T-4)-, tetrafluoroborate(1-) (9CI) (CA INDEX NAME)

CM 1

CRN 160473-36-9
CMF C62 H44 Cu N8 O2
CCI CCS





CM 2

CRN 14874-70-5
CMF B F4
CCI CCS

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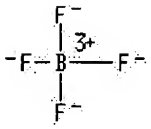
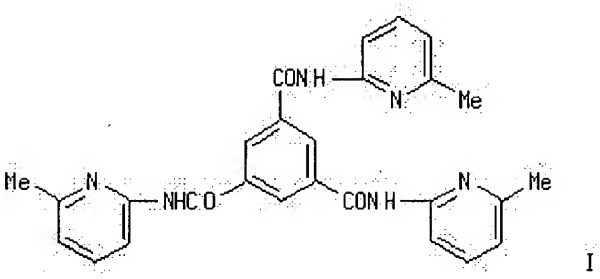


L12 ANSWER 115 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | More Like This | References

ACCESSION NUMBER: 1995:629812 HCAPLUS
DOCUMENT NUMBER: 123:32615
TITLE: Binding of Heptanedioic Acid to a Threefold Pyridine Arylamide Receptor. Enhancement of the Stability of Supramolecular Solution Structures by Multiple Binding Sites
AUTHOR(S): Koenig, Burkhard; Moeller, Oliver; Bubenitschek, Peter; Jones, Peter G.
CORPORATE SOURCE: Institut fuer Organische Chemie der Technischen, Universitaet Braunschweig, Braunschweig, D-38106, Germany
SOURCE: Journal of Organic Chemistry (1995), 60(13), 4291-3
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

AB Defined supramol. soln. structures with 1:1 stoichiometry were obtained from triamide I and heptanedioic acid (II) in chloroform, as shown by Jobs plot anal. of their 1H NMR spectra. A macroscopic binding const. for I and II was detd. as ≈2.5 105 ı L M-1. The incorporation of an addnl. binding moiety into I, compared to the previously reported diamide analog, results in a significant increase in the stability of the assembly arising from less restricted degrees of freedom. I was obtained from benzene-1,3,5-tricarbonyl chloride and 6-methyl-2-pyridinamine. The x-ray crystal structure anal. of I is reported.

IT **164174-81-6P**
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and binding with heptanedioic acid)
RN 164174-81-6 HCAPLUS
CN 1,3,5-Benzenetricarboxamide, N,N',N''-tris(6-methyl-2-pyridinyl)- (9CI) (CA INDEX NAME)

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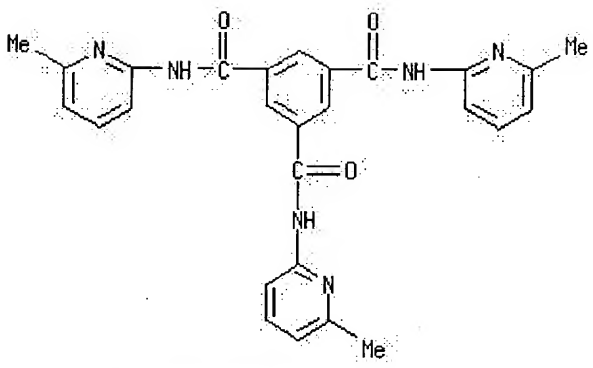


L12 ANSWER 116 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER:	1995:517657 HCAPLUS
DOCUMENT NUMBER:	123:32595
TITLE:	Molecular clefts derived from 9,9'-spirobi-9H-fluorene for enantioselective complexation of pyranosides and dicarboxylic acids
AUTHOR(S):	Cuntze, Jens; Owens, Linda; Alcazar, Victoria; Seiler, Paul; Diederich, Francois
CORPORATE SOURCE:	Lab. Org. Chem., Eidgenoessischen Tech. Hochschule, Zurich, CH-8092, Switz.
SOURCE:	Helvetica Chimica Acta (1995), 78(2), 367-90 CODEN: HCACAV; ISSN: 0018-019X
PUBLISHER:	Verlag Helvetica Chimica Acta
DOCUMENT TYPE:	Journal
LANGUAGE:	English
GI	

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The mol. clefts (R)- and (S)-I were prepd. via the bis(N-succinimidyl esters) of (R)- and (S)-9,9'-spirobi-9H-fluorene-2,2'-dicarboxylic acid. A spirobifluorene cleft with two different H-bonding sites (II) was also prepd. Binding studies with (R)- and (S)-I and optically active dicarboxylic acids in CDCl3 exhibited differences in free energy of the diastereoisomeric complexes formed; Δ(ΔG0) was 0.5-1.6 kcal mol-1 (300 K). Similar enantioselectivities were obsd. with the spirobifluorene clefts (R)- and (S)-III. The thermodn. quantities ΔH0 and ΔS0 for the recognition processes with (R)- and (S)-III were detd. by variable-temp. 1H-NMR titrns. and compared to those with (R)- and (S)-IV, contg. a conformationally more flexible 1,1'-binaphthyl moiety. All assocn. processes showed high enthalpic driving forces which are partially compensated for by unfavorable changes in entropy. Pyranosides bind to the optically active clefts III and I in CDCl3 with -ΔG0 = 3.0-4.3 kcal mol-1. Diastereoisomeric selectivities up to 1.2 kcal mol-1 and enantioselectivities up to 0.4 kcal mol-1 were obsd. Cleft II and N-(5,7-dimethyl-1,8-naphthyridin-2-yl)acetamide complexed pyranosides, e.g., V, as effectively as I, indicating that only one CONH(naphthyl) site in I assocs. strongly with the sugar derivs. Based on the x-ray crystal structure of I, a computer model for the complex between (S)-I and pyranoside V was constructed. Mol.-dynamics simulations showed that differential geometric constraints

h eb c g cg b cg eb

are at the origin of the high enantioselectivity in the complexation of dicarboxylic acid (S)-VI by (R)- and (S)-III and (R)- and (S)-I.

IT **143957-67-9P**

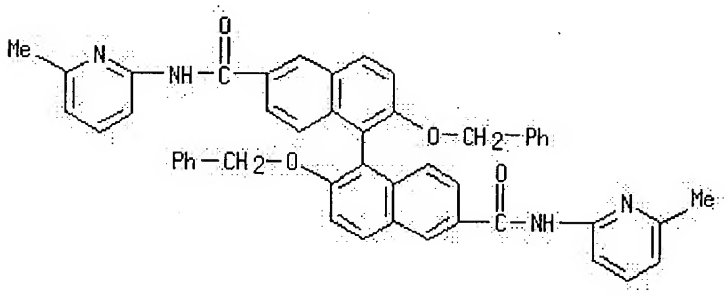
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (mol. clefts derived from spirobifluorene for enantioselective complexation of pyranosides and dicarboxylic acids)

RN 143957-67-9 HCAPLUS

CN L-Glutamic acid, N-[(phenylmethoxy)carbonyl]-, compd. with (R)-N,N'-bis(6-methyl-2-pyridinyl)-2,2'-bis(phenylmethoxy)[1,1'-binaphthalene]-6,6'-dicarboxamide (1:1) (9CI) (CA INDEX NAME)

CM 1

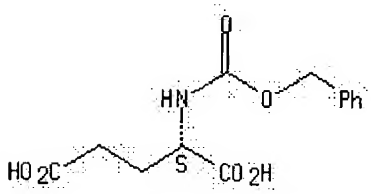
CRN 143957-66-8
CMF C48 H38 N4 O4



CM 2

CRN 1155-62-0
CMF C13 H15 N O6

Absolute stereochemistry.



L12 ANSWER 117 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Cited References

ACCESSION NUMBER:	1995:336118 HCAPLUS
DOCUMENT NUMBER:	122:285391
TITLE:	Synthetic hydrogen bonding receptors as models of transacylase enzymes
AUTHOR(S):	Tecilla, Paolo; Jubian, Vrej; Hamilton, Andrew D.
CORPORATE SOURCE:	Dep. of Chemistry, Univ. of Pittsburgh, Pittsburgh, PA, 15260, USA
SOURCE:	Tetrahedron (1995), 51(2), 435-48 CODEN: TETRAB; ISSN: 0040-4020
PUBLISHER:	Elsevier
DOCUMENT TYPE:	Journal
LANGUAGE:	English

AB A family of synthetic receptors has been prepd. contg. a barbiturate binding site and an appended thiol nucleophile. These are shown to cause large accelerations in the thiolysis reactions of barbiturate active ester

h eb c g cg b cg eb

derivs. The size of the acceleration is shown to depend critically on the length and flexibility of the spacer that links the thiol to the receptor.

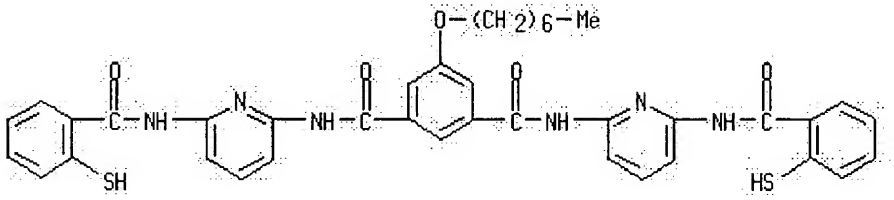
IT **131747-09-6P**

RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)

(enzyme model; synthetic hydrogen bonding receptors as models of transacylase enzymes)

RN 131747-09-6 HCAPLUS

CN 1,3-Benzenedicarboxamide, 5-(heptyloxy)-N,N'-bis[6-[(2-mercaptobenzoyl)amino]-2-pyridinyl]- (9CI) (CA INDEX NAME)



L12 ANSWER 118 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 1995:263058 HCAPLUS

DOCUMENT NUMBER: 122:105181

TITLE: A self-assembling receptor for dicarboxylic acids

AUTHOR(S): Goodman, M. Scott; Weiss, Jean; Hamilton, Andrew D.

CORPORATE SOURCE: Dep. of Chem., Univ. of Pittsburgh, Pittsburgh, PA, 15260, USA

SOURCE: Tetrahedron Letters (1994), 35(48), 8943-6
CODEN: TELEAY; ISSN: 0040-4039

PUBLISHER: Elsevier

DOCUMENT TYPE: Journal

LANGUAGE: English

AB In this paper we describe a simple binding subunit that self-assembles in the presence of metal ions to form a receptor for dicarboxylic acids. The resultant binding site is chiral and strong complexation to dicarboxylic acids in CDCl3 can be detected by both NMR and UV-vis spectroscopies.

IT **160473-38-1**

RL: FMU (Formation, unclassified); PRP (Properties); FORM (Formation, nonpreparative)

(self-assembling receptor for dicarboxylic acids)

RN 160473-38-1 HCAPLUS

CN Copper(1+), bis[N-(6-methyl-2-pyridinyl)-4-(9-phenyl-1,10-phenanthrolin-2-yl)benzamide-N4,N4']-, (T-4)-, tetrafluoroborate(1-), pentanedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 110-94-1
CMF C5 H8 O4

HO2C–(CH2)3–CO2H

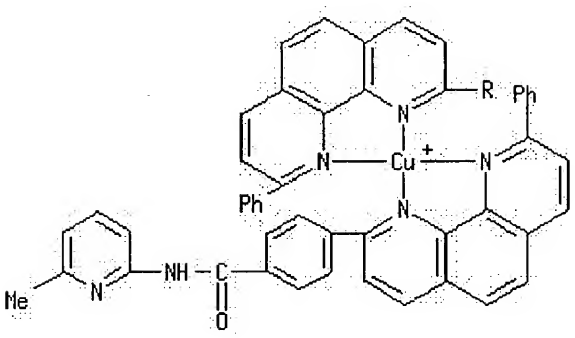
CM 2

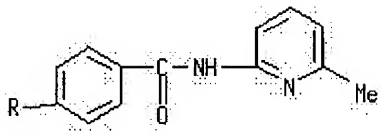
CRN 160473-37-0
CMF C62 H44 Cu N8 O2 . B F4

h eb c g cg b cg eb

CM 3

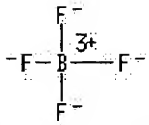
CRN 160473-36-9
CMF C62 H44 Cu N8 O2
CCI CCS





CM 4

CRN 14874-70-5
CMF B F4
CCI CCS



L12 ANSWER 119 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Shifts Parameters

ACCESSION NUMBER: 1995:71053 HCAPLUS
DOCUMENT NUMBER: 122:105008
TITLE: Intra- and intermolecular hydrogen bonding control of supramolecular structure
AUTHOR(S): Hamilton, Andrew D.; Hamuro, Yoshitomo; Yang, Ji; Geib, Steven J.; Fan, Erkang
CORPORATE SOURCE: Department Chemistry, University Pittsburgh, Pittsburgh, PA, 15260, USA
SOURCE: NATO ASI Series, Series C: Mathematical and Physical Sciences (1994), 426(COMPUTATIONAL APPROACHES IN SUPRAMOLECULAR CHEMISTRY), 101-8
CODEN: NSCSDW; ISSN: 0258-2023
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Hydrogen bonding is used to control supramol. structure in two distinct ways. The first involves intramol. hydrogen bonds to stabilize linear and helical conformations in synthetic oligomers. The second uses intermol.

h eb c g cg b cg eb

hydrogen bonding to direct the self-assembly of several interacting subunits.

IT **149540-94-3P**

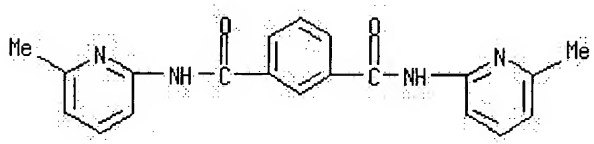
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (prepn. and hydrogen bonding of)

RN 149540-94-3 HCAPLUS

CN [1,1'-Biphenyl]-3,3'-dicarboxylic acid, compd. with N,N'-bis(6-methyl-2-pyridinyl)-1,3-benzenedicarboxamide (1:1) (9CI) (CA INDEX NAME)

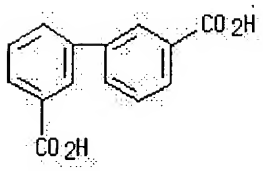
CM 1

CRN 130760-57-5
CMF C20 H18 N4 O2



CM 2

CRN 612-87-3
CMF C14 H10 O4



L12 ANSWER 120 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1994:655657 HCAPLUS
DOCUMENT NUMBER: 121:255657
TITLE: Preparation of bis(2-pyridylaminocarbonyl)benzene derivatives as fluorescent probes
INVENTOR(S): Aoki, Izu
o; Shinkai, Seiji
PATENT ASSIGNEE(S): Shingijutsu Kaihatsu Jigyodan, Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 14 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 06192224	A2	19940712	JP 1992-280674	19920926
JP 3027660	B2	20000404		

PRIORITY APPLN. INFO.: JP 1992-280674 19920926
OTHER SOURCE(S): MARPAT 121:255657
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

h eb c g cg b cg eb

AB Fluorescent compds. having fluorescent groups in a mol. skeleton to which a pair of 2-pyridylaminocarbonyl groups are bonded at a distance equiv. to 2-5 C atoms, preferably represented by a general formula (I; at least one of X1 - X3 = a group of atoms bonded to a fluorescent mol. and the others without being bonded to a fluorescent mol. = atom or a group of atoms not damaging the fluorescence property of the mol.), are prepd. I provide a suitable space between the 2-pyridylaminocarbonyl groups for capturing mols. having an ureido NHCONH or CO2H group, while the 2 NH groups and the N atoms of the 2 pyridine groups in I also serve as a site for capturing said mols. via hydrogen bonding, and the capturing of said mols. brings drastic change in the fluorescent property of the fluorescent group. By using these fluorescent compds. I as fluorescent probes, said mols. having an ureido or CO2H groups such as barbital- or hydantoin-related drugs (sedatives, tranquilizers, and anticonvulsants) are conveniently analyzed in high sensitivity and speed. Thus, 2,6-diaminopyridine was acylated by isophthaloyl dichloride in THF contg. Et3N to give 95% diamide (II; R = H) which was similarly acylated by 4-(1-pyrenyl)butyryl chloride (prepn. given) to give 71% II (R = Q4) (III). A soln. contg. 2.0 .times. 10-5 M barbital and 2 .times. 10-6 M III in CHCl3-cyclohexane showed fluorescence intensity from pyrene monomer (Im) of 119 at 380 nm and that of pyrene excimer (Iex) of 72 at .apprx.480 nm and Im/ex ratio of 2.29 vs. Im = 42, Iex = 72, and Im/Iex ratio = 0.58 in the absence of barbital.

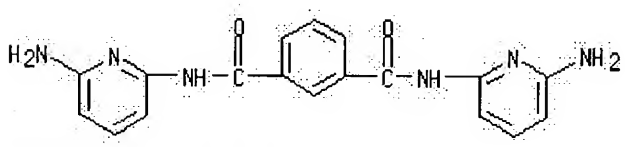
IT **112817-57-9P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(intermediate for prepn. of bis(pyridylaminocarbonyl)benzene derivs. as fluorescent probes for fluorescence anal.)

RN 112817-57-9 HCAPLUS

CN 1,3-Benzenedicarboxamide, N,N'-bis(6-amino-2-pyridinyl)- (9CI) (CA INDEX NAME)



L12 ANSWER 121 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER:	1994:557048 HCAPLUS
DOCUMENT NUMBER:	121:157048
TITLE:	Molecular recognition of cis-1,3,5-cyclohexanetricarboxylic acid
AUTHOR(S):	Ballester, Pablo; Costa, Antoni; Deya, Pere M.; Gonzalez, Jose F.; Rotger, M. Carmen; Deslongchamps, Ghislain
CORPORATE SOURCE:	Dep. de Quim., Univ. de les Illes Balears, Palma de Mallorca, 07071, Spain
SOURCE:	Tetrahedron Letters (1994), 35(22), 3813-16 CODEN: TELEAY; ISSN: 0040-4039
DOCUMENT TYPE:	Journal
LANGUAGE:	English

AB The design and synthesis of a new receptor, bearing amidopyridine units, designed to bind tricarboxylic acids in org. solvents is described. The properties of the complex formed between the new receptor and cis-1,3,5-cyclohexanetricarboxylic acid are studied.

IT **157460-61-2P**

h eb c g cg b cg eb

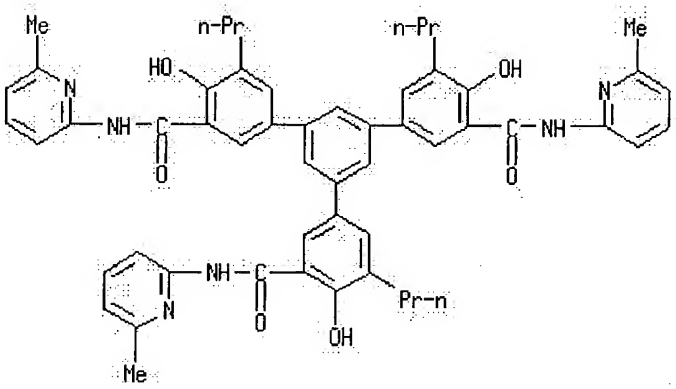
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and assocn. const. of)

RN 157460-61-2 HCAPLUS

CN 1,3,5-Cyclohexanetricarboxylic acid, (1α,3α,5α)-, compd. with 4,4''-dihydroxy-5'-[4-hydroxy-3-[[(6-methyl-2-pyridinyl)amino]carbonyl]-5-propylphenyl]-N,N'-bis(6-methyl-2-pyridinyl)-5,5''-dipropyl[1,1':3',1''-terphenyl]-3,3''-dicarboxamide (1:1) (9CI) (CA INDEX NAME)

CM 1

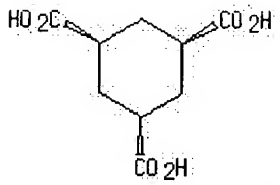
CRN 157460-60-1
CMF C54 H54 N6 O6



CM 2

CRN 16526-68-4
CMF C9 H12 O6

Relative stereochemistry.



L12 ANSWER 122 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

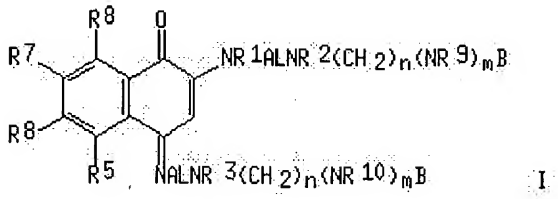
Full Text | Citing References

ACCESSION NUMBER:	1994:508263 HCAPLUS
DOCUMENT NUMBER:	121:108263
TITLE:	Preparation of N,N'-bis(sulfonamido)-2-amino-4-iminonaphthalen-1-ones and N,N'-bis(amido)-2-amino-4-iminonaphthalen-1-pnes
INVENTOR(S):	Defauw, Jean M.
PATENT ASSIGNEE(S):	Sphinx Pharmaceuticals Corp., USA
SOURCE:	U.S., 14 pp. CODEN: USXXAM
DOCUMENT TYPE:	Patent
LANGUAGE:	English
FAMILY ACC. NUM. COUNT:	1
PATENT INFORMATION:	

h eb c g cg b cg eb

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5292737	A	19940308	US 1992-965354	19921023
PRIORITY APPLN. INFO.:			US 1992-965354	19921023
OTHER SOURCE(S):	MARPAT 121:108263			

GI



I

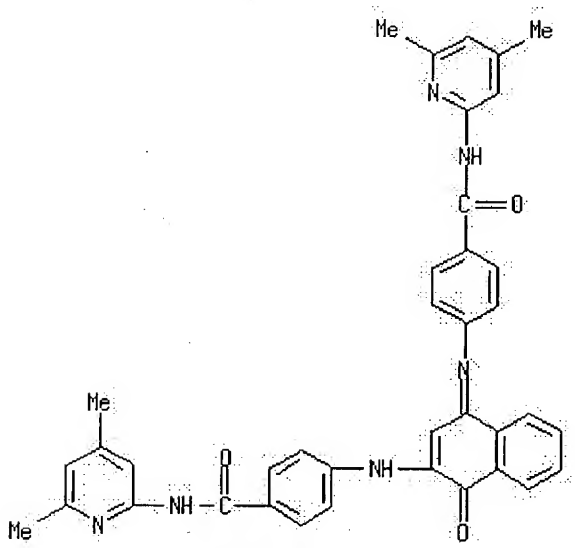
AB Title compds. I (A = Ph, naphthyl; L = O2S, CO; R1-3, R9,R10 = H, alkyl, aryl, alkylaryl, arylalkyl, cycloalkyl; R4-8 = H, alkyl, aryl, alkylaryl, arylalkyl, halo, O2N, (acyl) amino, HO, fused arom. ring, etc. B = H, aryl, arylalkyl, alkylaryl, C3-8 cycloalkyl, C2-20 alkenyl, C2-20 alkynyl acyl or substituted thereof, (substituted) heterocyclyl; m = 0,1; n = 0-6) or a salt thereof, inhibitors of protein kinase C and useful in treatment of inflammatory, cardiovascular and/or neplastic diseases, are prepd. To K 1,2-naphthoquinone-4-sulfonate in DMSO was added sulfamethoxazole to give I [R1-8 = H, A = Ph, L = SO2, m = n = 0, B = 3-(5-methylisoxazolyl)] (II). The IC50 of II in human tumor cell growth inhibition was 13.30 μM. I were evaluated for biol. activity as described above.

IT **156595-38-9P**

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of as drug)

RN 156595-38-9 HCAPLUS

CN Benzamide, N-(4,6-dimethyl-2-pyridinyl)-4-[[3-[[4-[[(4,6-dimethyl-2-pyridinyl)amino]carbonyl]phenyl]amino]-4-oxo-1(4H)-naphthalenylidene]amino]- (9CI) (CA INDEX NAME)



L12 ANSWER 123 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 1994:503388 HCAPLUS

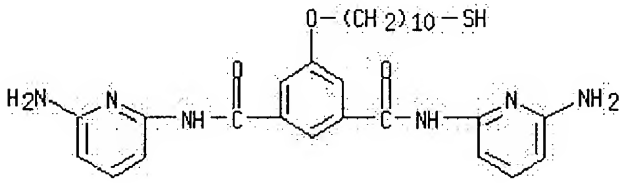
h eb c g cg b cg eb

DOCUMENT NUMBER: 121:103388
TITLE: Molecular Recognition in Membrane Mimics: A Fluorescence Probe
AUTHOR(S): Motesharei, Kianoush; Myles, David C.
CORPORATE SOURCE: Department of Chemistry and Biochemistry, University of California, Los Angeles, CA, 90024-1569, USA
SOURCE: Journal of the American Chemical Society (1994), 116(16), 7413-14
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A system is described for probing mol. recognition events in synthetic membranes using the change in the wavelength of fluorescence of receptors upon binding of ligand. The bis(2,6-diaminopyridine) amide of isophthalic acid was used as the receptor. Mixed monolayer contg. receptors functionalized with 10-carbon alkanethiol tethers and octanethiol were self-assembled on thin films of gold. A series of fluorescence expts. demonstrated that the presence of ligand by the receptor. The key evidence for interaction of the ligand and receptor was the reversible shift of the wavelength of fluorescence emission of the receptor in the presence and absence of the ligand.

IT **156946-14-4P**
RL: PREP (Preparation)
(prepn. of, for study of mol. recognition in membrane mimics)

RN 156946-14-4 HCAPLUS
CN 1,3-Benzenedicarboxamide, N,N'-bis(6-amino-2-pyridinyl)-5-[(10-mercaptodecyl)oxy]- (9CI) (CA INDEX NAME)



L12 ANSWER 124 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 1994:430454 HCAPLUS
DOCUMENT NUMBER: 121:30454
TITLE: Enhanced Extraction of Phenobarbital from Serum with a Designed Artificial Receptor
AUTHOR(S): Valenta, Jane N.; Dixon, Robert P.; Hamilton, Andrew D.; Weber, Stephen G.
CORPORATE SOURCE: Department of Chemistry, University of Pittsburgh, Pittsburgh, PA, 15260, USA
SOURCE: Analytical Chemistry (1994), 66(14), 2397-403
CODEN: ANCHAM; ISSN: 0003-2700
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The primary goal of this work was to det. whether artificial receptors that function on the basis of mol. recognition have anal. capabilities. As an example of such a receptor, the authors chose one directed toward barbiturates. Chloroform enriched with this artificial receptor (1 mM) can ext. more than 90% of the phenobarbital from a 20 μM phenobarbital soln. in human control serum using a vol. ratio (org./serum) as small as 0.5. In the absence of this receptor, the vol. ratio must be >10 to achieve similar extn. efficiencies. In addn. to vol. ratio, the role of

h eb c g cg b cg eb

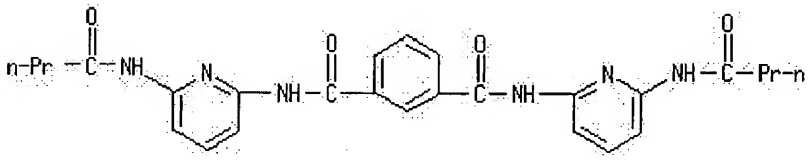
pH, receptor concn., and solvent type are discussed. The exptl. results are in good agreement with predictions based on chem. equil. Through the use of this and other similar receptors, the amt. of org. solvent used in extns. can be minimized.

IT **112817-60-4**

RL: ANST (Analytical study)
(barbiturate receptor, artificial)

RN 112817-60-4 HCAPLUS

CN 1,3-Benzenedicarboxamide, N,N'-bis[6-[(1-oxobutyl)amino]-2-pyridinyl]- (9CI) (CA INDEX NAME)

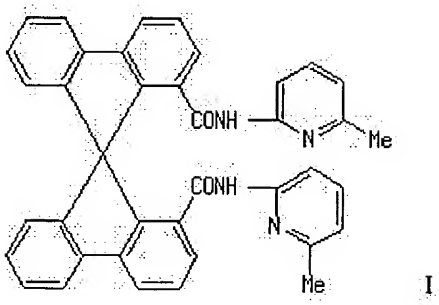


L12 ANSWER 125 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER:	1993:559608 HCAPLUS
DOCUMENT NUMBER:	119:159608
TITLE:	Enantioselective complexation of chiral dicarboxylic acids in 9,9'-spirobifluorene clefts
AUTHOR(S):	Alcazar, Victoria; Diederich, Francois
CORPORATE SOURCE:	Lab. Org. Chem., ETH Zent., Zurich, CH-8092, Switz.
SOURCE:	Anales de Quimica (1993), 89(1), 89-92 CODEN: ANQUEX; ISSN: 1130-2283
DOCUMENT TYPE:	Journal
LANGUAGE:	English

GI



I

AB The 9,9'-spirobifluorene receptors (R)- and (S)-I complex chiral dicarboxylic acids enantioselectively in chloroform via hydrogen bonding. A very large difference in stability, $\Delta(\Delta G^{\circ})$ = 1.8 kcal mol-1 was measured for the diastereomeric complexes formed by (R)- and (S)-I with a chiral 2,2'-dicarboxy-9,9'-spirobifluorene. In contrast, 1,1'-binaphthyl receptors with similar functionality in the major groove do not show significant enantioselectivity in the complexation of chiral dicarboxylic acids.

IT **143957-67-9**

RL: PROC (Process)
(formation const. and free energy of formation of)

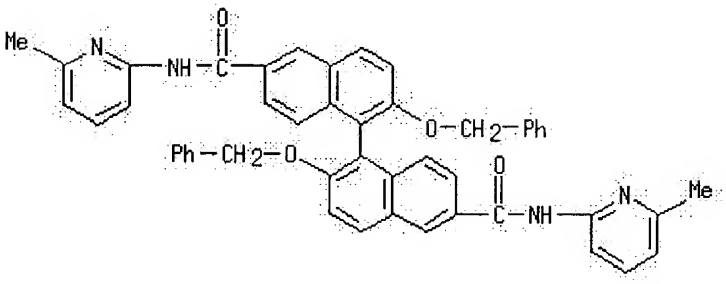
RN 143957-67-9 HCAPLUS

h eb c g cg b cg eb

CN L-Glutamic acid, N-[(phenylmethoxy)carbonyl]-, compd. with (R)-N,N'-bis(6-methyl-2-pyridinyl)-2,2'-bis(phenylmethoxy)[1,1'-binaphthalene]-6,6'-dicarboxamide (1:1) (9CI) (CA INDEX NAME)

CM 1

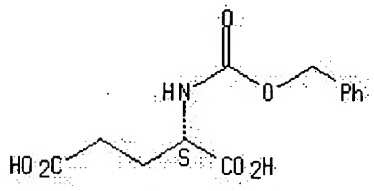
CRN 143957-66-8
CMF C48 H38 N4 O4



CM 2

CRN 1155-62-0
CMF C13 H15 N O6

Absolute stereochemistry.

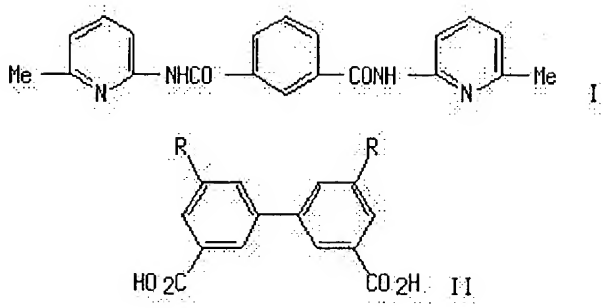


L12 ANSWER 126 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 1993:516712 HCAPLUS
DOCUMENT NUMBER: 119:116712
TITLE: Hydrogen-bonding control of molecular self-assembly: formation of a 2 + 2 complex in solution and in the solid state
AUTHOR(S): Yang, Ji; Fan, Erkang; Geib, Steven J.; Hamilton, Andrew D.
CORPORATE SOURCE: Mater. Res. Cent., Univ. Pittsburgh, Pittsburgh, PA, 15260, USA
SOURCE: Journal of the American Chemical Society (1993), 115(12), 5314-15
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

h eb c g cg b cg eb



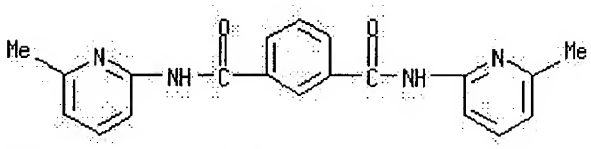
AB Two subunits of appropriate design, namely, I and II (R = H, CO2C10H21), can be induced to form, both in soln. and in the solid state, discrete 2 + 2 aggregates stabilized by a network of hydrogen bonds. The structure and stability of the aggregate were studied by x-ray crystallog., NMR, gel permeation chromatog. and vapor phase osmometry.

IT **130760-57-5**

RL: PRP (Properties)
(hydrogen bonding of, with biphenyldicarboxylic acids in soln. and solid state)

RN 130760-57-5 HCAPLUS

CN 1,3-Benzenedicarboxamide, N,N'-bis(6-methyl-2-pyridinyl)- (9CI) (CA INDEX NAME)

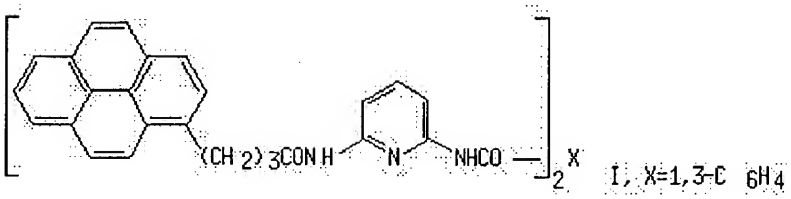


L12 ANSWER 127 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER:	1993:503501 HCAPLUS
DOCUMENT NUMBER:	119:103501
TITLE:	Molecular design of a new fluorescent barbiturate receptor. Sensitive detection of barbiturates through solvent extraction
AUTHOR(S):	Aoki, Izuo; Kawahara, Yohko; Sakaki, Toru; Harada, Takaaki; Shinkai, Seiji
CORPORATE SOURCE:	ERATO, Res. Dev. Corp., Kurume, 830, Japan
SOURCE:	Bulletin of the Chemical Society of Japan (1993), 66(3), 927-33 CODEN: BCSJA8; ISSN: 0009-2673
DOCUMENT TYPE:	Journal
LANGUAGE:	English

GI



h eb c g cg b cg eb

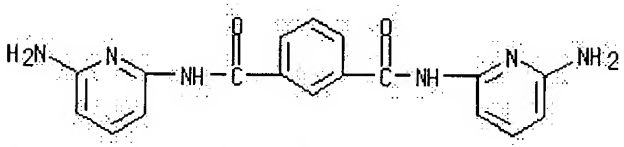
AB A fluorescent receptor, N,N'-bis[6-[4-(1-pyrenyl)butanamido]-2-pyridyl]isophthalamide (I), was synthesized to develop a sensitive host-guest-type sensory system for barbiturates. I aggregates in cyclohexane and the pyrene fluorescence in I almost disappeared because of aggregation-induced concn. quenching. The addn. of barbital to the cyclohexane soln. of I, which induced the deaggregation of I through complementary complexation with barbital, increased the fluorescence intensity at 378 nm by a factor of about 70-fold. The barbiturates in water could also be sensitively detected by I based on a liq. (water)-liq. (cyclohexane) extn. technique. In this system, I was essentially selective for barbiturates and no fluorescence response was obsd. for guests including a hydantoin skeleton. The analog of I, which has the N,N'-di-(2-pyridyl)terephthalamide skeleton, was also investigated as a fluorescent receptor for dicarboxylic acids.

IT **112817-57-9**

RL: RCT (Reactant); RACT (Reactant or reagent)
(acylation of, with pentanoyl chloride or pyrenylbutanoyl chloride)

RN 112817-57-9 HCAPLUS

CN 1,3-Benzenedicarboxamide, N,N'-bis(6-amino-2-pyridinyl)- (9CI) (CA INDEX NAME)



L12 ANSWER 128 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER:	1993:254302 HCAPLUS
DOCUMENT NUMBER:	118:254302
TITLE:	Molecular recognition of phosphate esters: a balance of hydrogen bonding and proton transfer interactions
AUTHOR(S):	Hirst, Simon C.; Tecilla, Paolo; Geib, Steven J.; Fan, Erkang; Hamilton, Andrew D.
CORPORATE SOURCE:	Dep. Chem., Univ. Pittsburgh, Pittsburgh, PA, 15260, USA
SOURCE:	Israel Journal of Chemistry (1992), 32(1), 105-11 CODEN: ISJCAT; ISSN: 0021-2148
DOCUMENT TYPE:	Journal
LANGUAGE:	English
OTHER SOURCE(S):	CASREACT 118:254302

AB The interaction of different phosphate esters with H-bonding receptors was examd. using UV, NMR, and x-ray crystallog. Crit. for binding is a combination of an acidic proton and the potential for bidentate H-bonding either between charged or uncharged components. Phosphotriesters show no binding to the receptors. Phosphodiesters bind to both bis(2,6-diacylaminopyridine) and mono-(2,6-diacylaminopyridine) receptors in chlorocarbon solvent via proton transfer to form the pyridinium phosphate ion pair and bidentate H-bonding between the anion and the cation. Titrn. expts. as well as Job's analyses show that for cyclic and acyclic bis(2,6-diacylaminopyridine) receptors 2:1 complexes are formed. Crystal structures demonstrate that in the solid state 2 different binding arrangements are present; either a direct bidentate interaction or intramol. H-bonding with self-assembly of an oligomeric structure. Phosphomonoesters bind to mono-(2,6-diacylaminopyridines) in a similar way to the diesters, via proton transfer and bidentate H-bonding. In this, as

h eb c g cg b cg eb

in the diester case, only a single acid-base interaction is possible and proton transfer is preferred. However, in the interaction of phosphomonoesters with bis(2,6-diacylaminopyridine) derivs. 2 acid-base interactions are possible between the two pyridines and two POH groups, and little proton transfer is seen. Strong binding (Ka = 1.0 105 ı M-1) occurs with the formation of 4 H-bonds. There is a balance between the occurrence of proton transfer and the no. of H-bonds formed between receptor and substrate.

IT **147767-91-7**

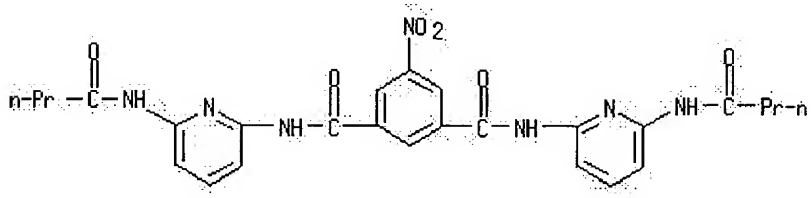
RL: PRP (Properties)
(UV and stoichiometry of)

RN 147767-91-7 HCAPLUS

CN Phosphoric acid, diphenyl ester, compd. with 5-nitro-N,N'-bis[6-[(1-oxobutyl)amino]-2-pyridinyl]-1,3-benzenedicarboxamide (1:1) (9CI) (CA INDEX NAME)

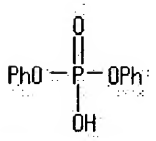
CM 1

CRN 129648-69-7
CMF C26 H27 N7 O6



CM 2

CRN 838-85-7
CMF C12 H11 O4 P

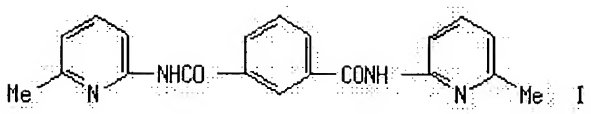


L12 ANSWER 129 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER:	1993:233397 HCAPLUS
DOCUMENT NUMBER:	118:233397
TITLE:	Self-organization to a helix via hydrogen-bridge bonds
AUTHOR(S):	Geib, Steven J.; Vicent, Cristina; Fan, Erkang; Hamilton, Andrew D.
CORPORATE SOURCE:	Mater. Res. Cent., Univ. Pittsburgh, Pittsburgh, PA, 15260, USA
SOURCE:	Angewandte Chemie (1993), 105(1), 85-5 (See also Angew. Chem., Int. Ed. Engl., 1993, 32(1), 80-1) CODEN: ANCEAD; ISSN: 0044-8249
DOCUMENT TYPE:	Journal
LANGUAGE:	German
GI	

h eb c g cg b cg eb



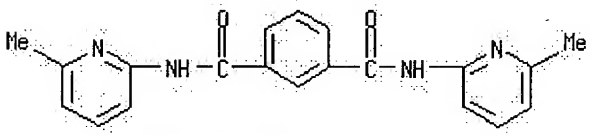
I

AB X-ray analyses of H-bridged polymeric 1:1 complexes of diamide I with heptane- and pentanedioic acid indicated helical chains. The conformations of the partners differed in the two complexes. The I-heptanedioic acid complex retained its helical structure in soln.

IT **130760-57-5**
RL: PRP (Properties)
(hydrogen bonding of, with heptanedioic and pentanedioic acid, helical complex by)

RN 130760-57-5 HCAPLUS

CN 1,3-Benzenedicarboxamide, N,N'-bis(6-methyl-2-pyridinyl)- (9CI) (CA INDEX NAME)



L12 ANSWER 130 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 1993:233206 HCAPLUS
DOCUMENT NUMBER: 118:233206
TITLE: Chiral molecular clefts for dicarboxylic acid complexation
AUTHOR(S): Alcazar, Victoria; Moran, Joaquin R.; Diederich, Francois
CORPORATE SOURCE: Dep. Chem. Biochem., Univ. California, Los Angeles, CA, 90024-1569, USA
SOURCE: Israel Journal of Chemistry (1992), 32(1), 69-77
CODEN: ISJCAT; ISSN: 0021-2148
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 118:233206
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *.

AB Three efficient cleft-type receptors, I-III are prepd. by attachment of 2 amidopyridine units as H-bonding centers to either the 2,2'-positions of 9,9'-spirobifluorene or the 6,6'-positions of 1,1'-binaphthyl spacers. The easy availability of these compds. in short synthetic routes make them attractive complexing agents for aliph. and arom. dicarboxylic acids which undergo bidentate binding in CHCl3. 1H NMR binding studies show that substrates of different size can be accommodated into the clefts and form 1:1 complexes that are predominantly stabilized by multiple host-guest H-bonds. The flexible aliph. substrates diethylmalonic, 2,2-diphenylsuccinic, glutaric, and pimelic acid form complexes with assocn. consts. Ka ranging from 103 to 104 L mol-1. Significantly more stable complexes (Ka > 105 L mol-1) are obtained with the more rigid,

h eb c g cg b cg eb

preorganized substrate 5-dodecyloxyisophthalic acid.

IT **147650-11-1**

RL: PRP (Properties)
(formation const. of)

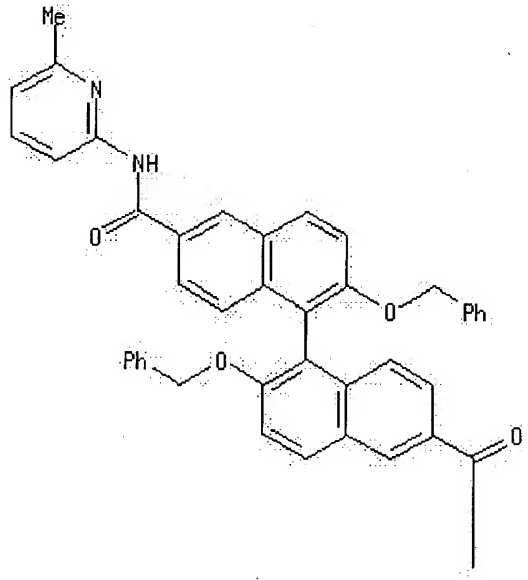
RN 147650-11-1 HCAPLUS

CN Butanedioic acid, 2,2-diphenyl-, compd. with N,N'-bis(6-methyl-2-pyridinyl)-2,2'-bis(phenylmethoxy)[1,1'-binaphthalene]-6,6'-dicarboxamide (1:1) (9CI) (CA INDEX NAME)

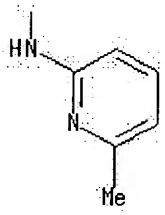
CM 1

CRN 147650-10-0
CMF C48 H38 N4 O4

PAGE 1-A

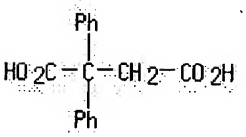


PAGE 2-A



CM 2

CRN 10186-26-2
CMF C16 H14 O4



L12 ANSWER 131 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

h eb c g cg b cg eb

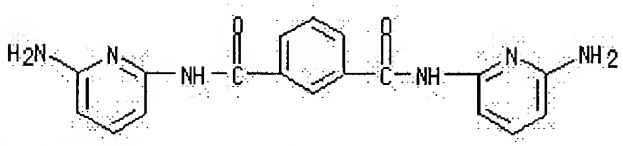
Full Text | Citing References

ACCESSION NUMBER: 1993:208282 HCAPLUS
DOCUMENT NUMBER: 118:208282
TITLE: Molecular reception catalysis of the decarboxylation of N-carboxyimidazolidinone. A model for activation by distortion of N-carboxybiotin
AUTHOR(S): Kluger, Ronald; Tsao, Belinda
CORPORATE SOURCE: Dep. Chem., Univ. Toronto, Toronto, ON, M5S 1A1, Can.
SOURCE: Journal of the American Chemical Society (1993), 115(5), 2089-90
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The decarboxylation of enzyme-bound N-carboxybiotin is induced by the binding of substrates and substrate analogs. The induction has been proposed to result from movement of the carboxyl group of N-carboxybiotin out of the plane of the imidazolidinone ring as a result of binding interactions with the protein. A macrocyclic host, (H), was designed to be complementary to imidazolidinone while its assocn. with N-carboxyimidazolidinone (I) will have steric interactions which should lead to distortion toward the transition state for decarboxylation. Kinetic anal. (25 °, tetrahydrofuran) shows that H is a specific and effective catalyst for the decarboxylation of I.

IT **112817-57-9**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with diacid dichloride)

RN 112817-57-9 HCAPLUS
CN 1,3-Benzenedicarboxamide, N,N'-bis(6-amino-2-pyridinyl)- (9CI) (CA INDEX NAME)



L12 ANSWER 132 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

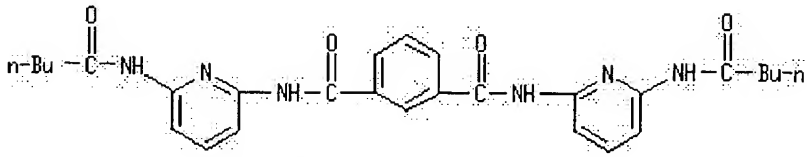
ACCESSION NUMBER: 1993:21861 HCAPLUS
DOCUMENT NUMBER: 118:21861
TITLE: Fluorescence reading-out of the molecular-recognition process
AUTHOR(S): Aoki, Izuo; Harada, Takaaki; Sakaki, Toru; Kawahara, Yohko; Shinkai, Seiji
CORPORATE SOURCE: Fukuoka Ind. Technol. Cent., Chikushino, 818, Japan
SOURCE: Journal of the Chemical Society, Chemical Communications (1992), (18), 1341-5
CODEN: JCCCAT; ISSN: 0022-4936
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The binding of guest mols. sensitively influences the fluorescent behavior of barbiturate-incorporated fluorescent pyrenes, making it possible to read out the mol.-recognition process by a fluorescence spectroscopic technique.

IT **144918-26-3**
RL: PRP (Properties)
(NMR of, barbiturate effect on)

h eb c g cg b cg eb

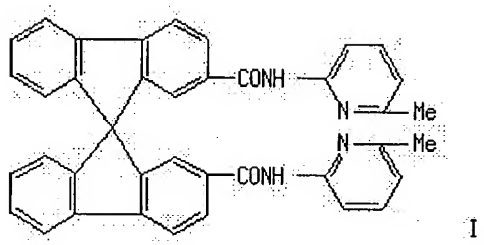
RN 144918-26-3 HCAPLUS
CN 1,3-Benzenedicarboxamide, N,N'-bis[6-[(1-oxopentyl)amino]-2-pyridinyl]-(9CI) (CA INDEX NAME)



L12 ANSWER 133 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Chem Refs

ACCESSION NUMBER: 1993:6571 HCAPLUS
DOCUMENT NUMBER: 118:6571
TITLE: Enantioselective complexation of chiral dicarboxylic acids in functionalized split 9,9'-spirobifluorenes
AUTHOR(S): Alcazar, Victoria; Diederich, Francois
CORPORATE SOURCE: Lab. Org. Chem., ETH-Zent., Zurich, CH-8092, Switz.
SOURCE: Angewandte Chemie (1992), 104(11), 1503-5 (See also Angew. Chem., Int. Ed. Engl., 1992, 31(11), 1521-3)
CODEN: ANCEAD; ISSN: 0044-8249
DOCUMENT TYPE: Journal
LANGUAGE: German
GI



I

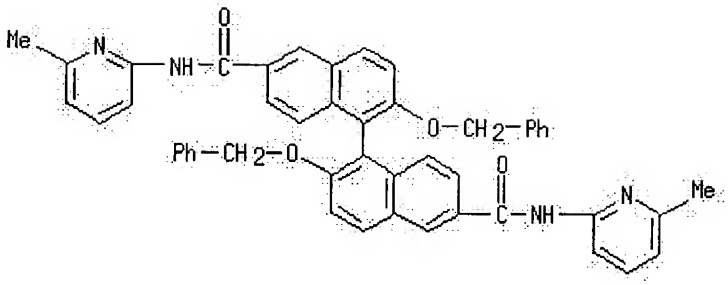
AB Enantioselective complexation of chiral dicarboxylic acids, e.g., (S)-PhCH2OCONHCH(CO2H)CH2CO2H, with (R)- and (S)-I was examd. I showed higher potential than similar 1,1'-binaphthyls for differentiating enantiomers.

IT **143957-67-9**
RL: PROC (Process)
(formation const. and free energy of formation of)
RN 143957-67-9 HCAPLUS
CN L-Glutamic acid, N-[(phenylmethoxy)carbonyl]-, compd. with (R)-N,N'-bis(6-methyl-2-pyridinyl)-2,2'-bis(phenylmethoxy)[1,1'-binaphthalene]-6,6'-dicarboxamide (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 143957-66-8
CMF C48 H38 N4 O4

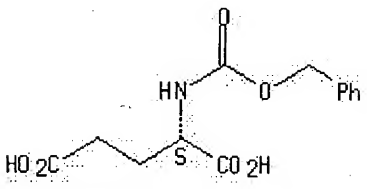
h eb c g cg b cg eb



CM 2

CRN 1155-62-0
CMF C13 H15 N O6

Absolute stereochemistry.



L12 ANSWER 134 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

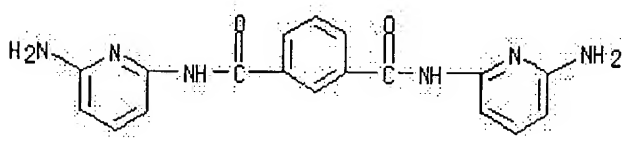
Full Text | CAPLUS References

ACCESSION NUMBER: 1992:605053 HCAPLUS
DOCUMENT NUMBER: 117:205053
TITLE: Molecular recognition: porphyrin-containing receptors as analogs of barbiturate-induced cytochrome P450
AUTHOR(S): Slobodkin, Gregory; Fan, Erkang; Hamilton, Andrew D.
CORPORATE SOURCE: Dep. Chem., Univ. Pittsburgh, Pittsburgh, PA, 15260, USA
SOURCE: New Journal of Chemistry (1992), 16(5), 643-5
CODEN: NJCHE5; ISSN: 0398-9836
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The synthesis and complexation properties of a porphyrin-contg. receptor for barbiturates are reported. 1H NMR methods are used to study the interaction of different barbiturates with the receptor and the structure of the complex is shown to be dependent on the size of substituents in the 5,5-positions. Complexation places the substrate directly above the porphyrin ring and the possible similarity of this arrangement to the active site of barbiturate-induced cytochrome P 450 is discussed.

IT **112817-57-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and reaction of, with porphyrin deriv.)

RN 112817-57-9 HCAPLUS
CN 1,3-Benzenedicarboxamide, N,N'-bis(6-amino-2-pyridinyl)- (9CI) (CA INDEX NAME)



h eb c g cg b cg eb

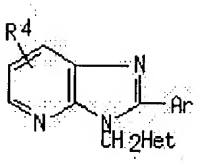
L12 ANSWER 135 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 1992:448553 HCAPLUS
DOCUMENT NUMBER: 117:48553
TITLE: Preparation of 2-aryl-3-(heterocyclylmethyl)-3H-imidazo[4,5-b]pyridines as anxiolytics and anticonvulsants
INVENTOR(S): Taylor, Chandler R., Jr.; Moses, Meredith
PATENT ASSIGNEE(S): A. H. Robins Co., Inc., USA
SOURCE: U.S., 8 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5066654	A	19911119	US 1990-601967	19901022
PRIORITY APPLN. INFO.:			US 1990-601967	19901022

OTHER SOURCE(S): MARPAT 117:48553
GI



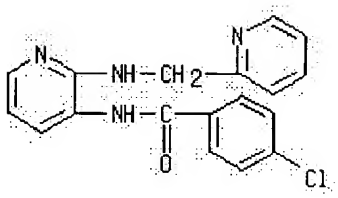
I

AB Title compds. I [Ar = (substituted) Ph, (substituted) pyridyl; Het = (substituted) imidazolyl, (substituted) oxazolyl, (substituted) pyrimidyl, (substituted) thiazolyl; R4 = H, C16 alkyl, C7-10 aralkyl, C1-6 alkoxy, C2-7 carbalkoxy, halo F3C] or a salt thereof, are prepd. To a stirred soln. of 2-chloro-3-nitropyridine in EtOH were added 2-(aminomethyl)pyridine and Et3N and and the resulting mixt. was refluxed for 2 h to give N-(3-nitro-2-pyridinyl)-2-pyridinemmethanamine, which was hydrogenated in THF over 5% Pd/charcoal followed by treatment with 4-chlorobenzamide to give 4-chloro-N-[2-[(2-pyridinylmethyl)amino]-3-pyridinyl]benzamide which was refluxed with HOCH2CH2OH for 1.5 h, then stirred at room temp. overnight to give I (Ar = 4-ClC6H4, Het = 2-pyridyl, R4 = H)(II). In an in vitro test, II had an IC50 of 7000 nM in inhibiting [3H]-flunitrazepam binding.

IT **138824-02-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and reaction of, in prepn. of anticonvulsants and anxiolytics)

RN 138824-02-9 HCAPLUS
CN Benzamide, 4-chloro-N-[2-[(2-pyridinylmethyl)amino]-3-pyridinyl]- (9CI) (CA INDEX NAME)

h eb c g cg b cg eb

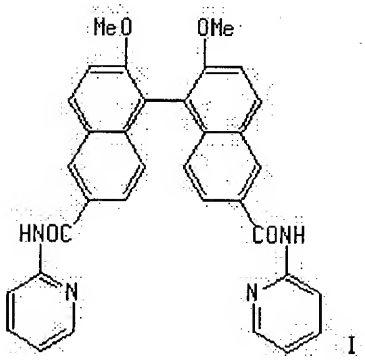


L12 ANSWER 136 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | More References

ACCESSION NUMBER:	1992:105783 HCAPLUS
DOCUMENT NUMBER:	116:105783
TITLE:	Chiral recognition of tartaric acid derivatives by a synthetic receptor
AUTHOR(S):	Garcia-Tellado, Fernando; Albert, Jeffrey; Hamilton, Andrew D.
CORPORATE SOURCE:	Dep. Chem., Univ. Pittsburgh, Pittsburgh, PA, 15260, USA
SOURCE:	Journal of the Chemical Society, Chemical Communications (1991), (24), 1761-3 CODEN: JCCCAT; ISSN: 0022-4936
DOCUMENT TYPE:	Journal
LANGUAGE:	English

GI



AB A synthetic receptor (I) contg. two acylaminopyridine groups linked through an R-(-)-binaphthyl spacer was prepd. and shown to bind to the two enantiomeric forms of diacyl tartaric acids by two very different geometries.

IT **139097-80-6P**

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (prepn. and NMR of)

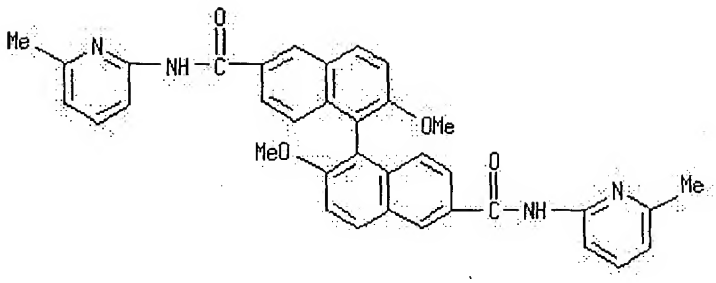
RN 139097-80-6 HCAPLUS

CN Butanedioic acid, 2,3-bis(benzoyloxy)-, [S-(R*,R*)]-, compd. with (R)-2,2'-dimethoxy-N,N'-bis(6-methyl-2-pyridinyl)[1,1'-binaphthalene]-6,6'-dicarboxamide (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 139097-79-3

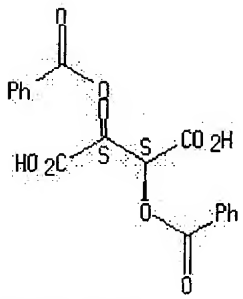
CMF C36 H30 N4 O4



CM 2

CRN 17026-42-5
CMF C18 H14 O8

Absolute stereochemistry. Rotation (+).



L12 ANSWER 137 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | More References

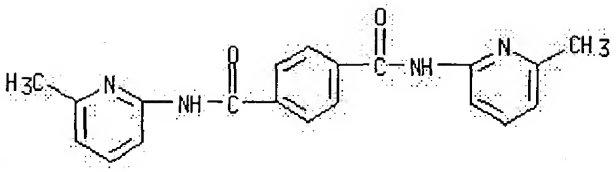
ACCESSION NUMBER: 1992:5992 HCAPLUS
DOCUMENT NUMBER: 116:5992
TITLE: Complexation control of pericyclic reactions: supramolecular effects on the intramolecular Diels-Alder reaction [Erratum to document cited in CA114(3):23229t]
AUTHOR(S): Hirst, Simon C.; Hamilton, Andrew D.
CORPORATE SOURCE: Dep. Chem., Univ. Pittsburgh, Pittsburgh, PA, 15260, USA
SOURCE: Journal of the American Chemical Society (1991), 113(19), 7449
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: English

AB An error in footnote 16 has been cor. The error was not reflected in the abstr. or the index entries.

IT 129708-38-9
RL: PRP (Properties)
(effect of, on intramol. Diels-Alder reaction of furfurylfumaramide (Erratum))

RN 129708-38-9 HCAPLUS
CN 1,4-Benzenedicarboxamide, N,N'-bis(6-methyl-2-pyridinyl)- (9CI) (CA INDEX NAME)

h eb c g cg b cg eb



L12 ANSWER 138 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Other References

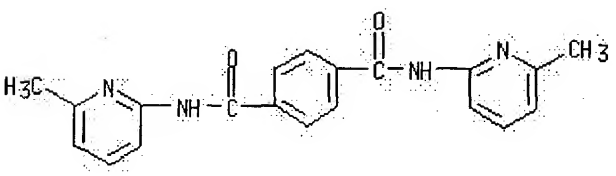
ACCESSION NUMBER: 1991:667282 HCAPLUS
DOCUMENT NUMBER: 115:267282
TITLE: Molecular recognition in the solid state: controlled assembly of hydrogen-bonded molecular sheets
AUTHOR(S): Garcia-Tellado, Fernando; Geib, Steven J.; Goswami, Shyamaprosad; Hamilton, Andrew D.
CORPORATE SOURCE: Dep. Chem., Univ. Pittsburgh, Pittsburgh, PA, 15260, USA
SOURCE: Journal of the American Chemical Society (1991), 113(24), 9265-9
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A novel H-bonding motif for the control of solid-state structures was deeloped. The motif is based on the H bonding complementarity of carboxylic acids with 2-aminopyridine derivs. Linking 2 aminopyridine groups through a rigid arom. spacer provides a receptor unit that can complex dicarboxylic acids. When there is a good correspondence between the length of the spacer tna that of the carboxylic acid, a discrete 1:1 complex is formed. When the dicarboxylic acid is longer than the receptor, an alternating H-bonded cocrystal occurs with the carboxylates on each diacid binding to different receptors. This motif dominates the cocrystal, forming even when the relative lengths of the diacid and the receptor change. Within the constraints of the alternating ribbon structure, the spatial position of the 2 components can be varied in a well-defined and predictable manner. Crystallog. data for the 2-aminopyridine deriv.-dicarboxylic acid complexes are given.

IT **129708-39-0**
RL: PRP (Properties)
(crystal structure of)
RN 129708-39-0 HCAPLUS
CN Hexanedioic acid, compd. with N,N'-bis(6-methyl-2-pyridinyl)-1,4-benzenedicarboxamide (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 129708-38-9
CMF C20 H18 N4 O2



CM 2

CRN 124-04-9

h eb c g cg b cg eb

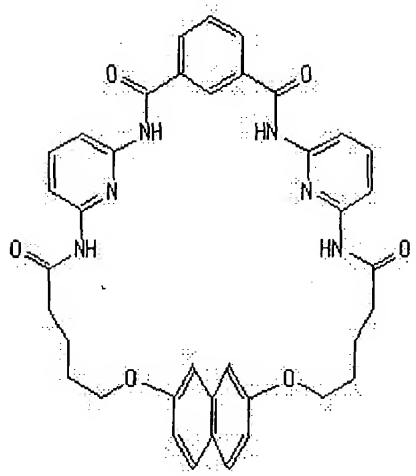
CMF C6 H10 O4

HO2C-(CH2)4-CO2H

L12 ANSWER 139 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Other References

ACCESSION NUMBER: 1991:559114 HCAPLUS
DOCUMENT NUMBER: 115:159114
TITLE: Hydrogen bonding and molecular recognition: synthetic, complexation, and structural studies on barbiturate binding to an artificial receptor
AUTHOR(S): Chang, Suk Kyu; Van Engen, Donna; Fan, Erkang; Hamilton, Andrew D.
CORPORATE SOURCE: Dep. Chem., Univ. Pittsburgh, Pittsburgh, PA, 15260, USA
SOURCE: Journal of the American Chemical Society (1991), 113(20), 7640-5
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



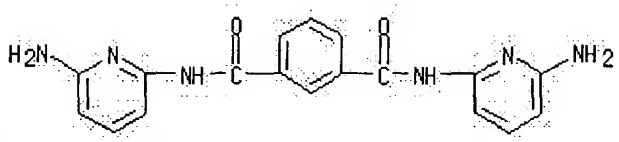
I

AB A series of synthetic receptors, e.g., I, with strong selectivity for the barbiturate family of drugs has been prepd. The receptor design is based on two 2,6-diaminopyridine groups linked through an isophthalic acid spacer. X-ray crystallog., 1H NMR spectroscopic, and substrate binding studies confirm that six hydrogen bonds are formed between the receptor and its substrate. The strongest binding (Ka ~ 105M-1) is seen to those substrates contg. the complementary barbituric acid core. Systematic deletion of hydrogen-bonding sites from the receptor and substrate allows an assessment of the contribution of individual binding sites to complexation.

IT **112817-57-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and macrocyclization of, with naphthalenediol or bis[(chlorocarbonylpropyloxy)phenyl]propane)

h eb c g cg b cg eb

RN 112817-57-9 HCAPLUS
CN 1,3-Benzenedicarboxamide, N,N'-bis(6-amino-2-pyridinyl)- (9CI) (CA INDEX NAME)



L12 ANSWER 140 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

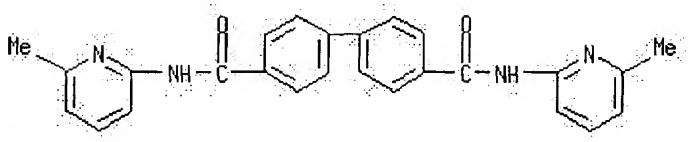
Full Text | CHNG References

ACCESSION NUMBER: 1991:429867 HCAPLUS
DOCUMENT NUMBER: 115:29867
TITLE: Conformational selectivity in molecular recognition: the influence of artificial receptors on the cis-trans isomerization of acylprolines
AUTHOR(S): Vicent, Cristina; Hirst, Simon C.; Garcia-Tellado, Fernando; Hamilton, Andrew D.
CORPORATE SOURCE: Dep. Chem., Univ. Pittsburgh, Pittsburgh, PA, 15260, USA
SOURCE: Journal of the American Chemical Society (1991), 113(14), 5466-7
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The cis-trans isomerization of acylprolines is a process of great importance in biochem. In this paper a study of the effect of different artificial receptors on the rotamer equil. of a series of proline diacids is reported. Receptors with appropriately positioned carboxylate binding groups can selectively bind to one of the two rotamers and influence the equil. by up to 32-fold.

IT **134418-77-2**
RL: RCT (Reactant); RACT (Reactant or reagent)
(conformational equil. of acylproline deriv. in presence of)

RN 134418-77-2 HCAPLUS
CN [1,1'-Biphenyl]-4,4'-dicarboxamide, N,N'-bis(6-methyl-2-pyridinyl)- (9CI) (CA INDEX NAME)



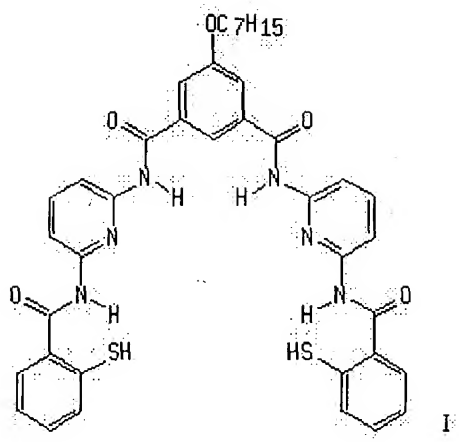
L12 ANSWER 141 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | CHNG References

ACCESSION NUMBER: 1991:80754 HCAPLUS
DOCUMENT NUMBER: 114:80754
TITLE: Molecular recognition and catalysis: acceleration of acyl-transfer reactions by a hydrogen-bonding receptor
AUTHOR(S): Tecilla, Paolo; Hamilton, Andrew D.
CORPORATE SOURCE: Dep. Chem., Univ. Pittsburgh, Pittsburgh, PA, 15260, USA
SOURCE: Journal of the Chemical Society, Chemical Communications (1990), (18), 1232-4

h eb c g cg b cg eb

CODEN: JCCCAT; ISSN: 0022-4936
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 114:80754
GI

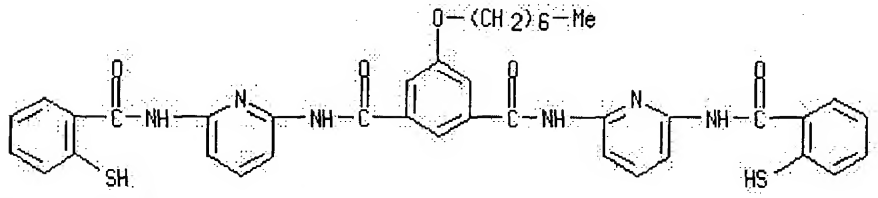


I

AB An H-bonding receptor contg. an appended thiol (I) was synthesized and shown to cause large rate accelerations (kobs/kuncat >104) in the thiolysis reaction of complementary barbiturate acetate derivs.

IT **131747-09-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, as hydrogen-bonding receptor, acceleration of acyl transfer reactions by)

RN 131747-09-6 HCAPLUS
CN 1,3-Benzenedicarboxamide, 5-(heptyloxy)-N,N'-bis[6-[(2-mercaptobenzoyl)amino]-2-pyridinyl]- (9CI) (CA INDEX NAME)



L12 ANSWER 142 OF 162 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Cited References

ACCESSION NUMBER: 1991:23229 HCAPLUS
DOCUMENT NUMBER: 114:23229
TITLE: Complexation control of pericyclic reactions: supramolecular effects on the intramolecular Diels-Alder reaction
AUTHOR(S): Hirst, Simon C.; Hamilton, Andrew D.
CORPORATE SOURCE: Dep. Chem., Univ. Pittsburgh, Pittsburgh, PA, 15260, USA
SOURCE: Journal of the American Chemical Society (1991), 113(1), 382-3
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal

h eb c g cg b cg eb